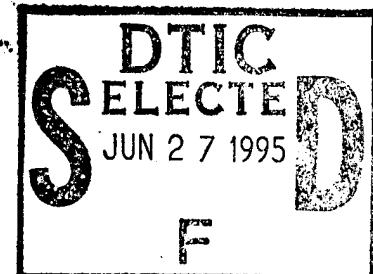


**PL-TR-95-2060(II)**  
**Special Reports, No. 274**

**PROCEEDINGS OF THE 17TH ANNUAL  
CONFERENCE ON ATMOSPHERIC  
TRANSMISSION MODELS,  
8-9 JUNE 1994**

**Editors:**

**Gail P. Anderson  
Richard H. Picard  
James H. Chetwynd**



**24 May 1995**

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AIR FORCE MATERIEL COMMAND  
HANSCOM AFB, MA 01731-3010**

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"This technical report has been reviewed and is approved for publication"

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**Synthetic 3-D Atmospheric Temperature Structure:  
A Model for Known Geophysical Power Spectra Using  
A Hybrid Autoregression And Fourier Technique**

James H. Brown  
Neil Grossbard



**SYNTHETIC 3-D ATMOSPHERIC TEMPERATURE STRUCTURE: A  
MODEL FOR KNOWN GEOPHYSICAL POWER SPECTRA USING A  
HYBRID AUTOREGRESSION AND FOURIER TECHNIQUE**

James H. Brown  
Neil Grossbard

**Abstract**

Within a defined domain, geophysical phenomena often are characterized by smooth continuous power spectral densities having a negative power law slope dependence. Frequently, Fourier transform analysis has been employed to generate synthetic scenes from pseudorandom arrays by passing the stochastic data through a Fourier filter having a desired correlation structure and power spectral dependency. This report examines the possibility of producing synthetic structure by invoking autoregression analysis in conjunction with the Fourier method. Since computations that apply multidimensional fast Fourier transforms to large data arrays consume enormous resources and time, the goal of this study is to seek an alternative method to reduce the computational burden. Future editions of the Phillips Laboratory Atmospheric Radiance Codes will feature an ability to calculate structured radiance. The methods explored herein provide a process that can complement or in some cases supplement methods presently being used. Line of sight computations using the three-dimensional database will be presented.

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Memo

Figures

1. Title Page
2. Stepping Stones - References from previous work
3. Linear Difference Equation - An autoregressive moving average (ARMA) model for a discrete spatial series,  $v(n)$ , that approximates deterministic and stochastic processes can be represented by the filter linear difference equation:
4. Power Spectra Model - A z transform analysis of the difference equation shows that the ARMA power spectral density ( $P_{ARMA}(k)$ ) is contained in the equations in the slide.
5. Yule-Walker Equations - The relationship between the autocorrelation sequence and the pure autoregressive model is contained in the equations in the slide.
6. Levinson Recursion Algorithm - A standard "Levinson" algorithm that takes advantage of the Hermitian-Toeplitz matrix equation was employed to solve for the AR parameters. These are presented in the equations in the slide.
7. PSD of Simulated Series - the simulated PSD is obtained from the formula given in the slide. For a given altitude, the forward and backward method solves the squares problem given in the slide.
8. PSD and ACF Models - In practice, a given one-dimensional *single-sided* PSD was constructed from the PSD and ACF power law models as shown in the slide.
9. Coherence Length Parameter - the equivalent width or correlation length as a function of the PSD may be written as presented in the slide.

Memo

10. PSD - The model autocorrelation function used in this report leads to an isotropic two-dimensional power spectral density function given by the equation in the slide. The simulated data,  $S(t, \ell)$ , for a layer is described by the second equation in the slide.
11. Transverse Correction - In pursuit of avoiding the time-consuming convolution integral, an approximation was developed that modified the  $PSD(k_t, k_\ell)$  at  $k_t = 0$ . This is given by the equation in the slide. The horizontal two-dimensional discrete Fourier Transform used in the syntheses of the database results in a well-known rectangular window sampling effect. Assuming negligible truncation of the autocorrelation function in the line-of-sight direction, truncation in the transverse direction leads to side-lobe leakage of the frequency response function of the digitized rectangular window. In the transverse direction, the effects of leakage can be computed as the convolution of the "theoretical"  $PSD(k_t, k_\ell)$  with the square of the magnitude of the frequency response of a digital sinc function.
12. Line-of Sight Correction - Since the constructed database has a finite and relatively large line-of-sight data spacing, a natural truncation of the line-of-sight power spectral density function must occur that would cause significant aliasing of the line-of-sight PSD's for any particular realization. Computational "aliasing" of the line-of-sight PSD's was added to the "theoretical" PSD's by the equations in the slide.
13. Conclusions Slide. Self-contained

## Backup Table

It is anticipated that the following Table will be presented in answer to questions.

1. The chosen geometry is a segment of a sphere that consists of a volume 70 km in height by approximately 3000 km in the sensor LOS direction by approximately 51.2 km in the direction transverse to the line-of-sight. A spatial resolution element has an incremental altitude of 0.1 km by an incremental transverse distance of approximately 0.1 km by an incremental LOS distance of approximately 15.7 km. The actual data spacing in the horizontal dimension increased slightly with altitude so that points in the vertical dimension stayed on radial lines. The altitude range accounts for dominant structure effects (50-120 km). Also its vertical and transverse dimensions are sufficient to fill the field of a limb-viewing two-dimensional sensor array. The vertical and transverse spatial resolution is governed by the vertical and horizontal correlation lengths of the temperature variations but also is chosen to provide high field-of-view spatial resolution. The geometrical LOS dimensions are chosen to provide sufficient length to describe the integrated path radiance. Table 1 summarizes the database specifications.

## Backup Figures

It is anticipated that the following Figures will be presented in answers to questions.

1. Database Geometry. Figure 1a illustrates the volume of the spherical segment defined by the database. The radial altitude range starts at 50 km and ends at 120 km. At 50 km altitude the curved length in the LOS direction measures 3014 km while the curved length in the transverse direction measures 51.2 km. These distances increase slightly with altitude due to the curved geometry. Figure 1b illustrates the resolution volume at 50 km. The radial altitude resolution is 0.1 km while the resolution of the curved lengths in the LOS and transverse directions is 15.7 km and 0.1 km respectively. Again the horizontal resolution lengths increase slightly with altitude.
2. Computational scheme. Correlations along the vertical lines are calculated (one layer at a time) and then the horizontal correlation calculation is applied to each layer.
3. Horizontal correlation lengths plotted as a function of altitude. A logistic dose response equation is fitted to the data. The outside curves represent the 95% confidence limits.
4. Vertical correlation lengths plotted as a function of altitude. A logistic dose response equation is fitted to the data. The outside curves represent the 95% confidence limits.
5. Root mean square values of the relative temperature fluctuations plotted as a function of altitude. A rational polynomial is fitted to the data. The outside curves represent the 95% confidence limits.
6. Graphs of Vertical, Transverse, and Line-of-Sight one-dimensional Power Spectral Densities plotted against spatial frequency. The left panel plots the vertical *PSD*'s for the theoretical model (light gray solid curve), autoregressive "generator" model (dashed curve), and the autoregressive vertical *PSD* from the simulated database (dotted curve). The middle panel plots the transverse *PSD*'s for the theoretical model (light gray solid curve), autoregressive *PSD* from the simulated database (dotted curve), and a periodogram from the simulated database (solid curve). The right panel plots the line-of-sight *PSD*'s for the theoretical model (light gray solid curve), autoregressive *PSD* from the simulated database (dotted curve), and a periodogram from the simulated database (solid curve). The plots are for 50.6 km altitude and one-dimensional high frequency spectral slope ( $S$ ) =  $-5/3$ , where  $\sigma^2 = 8.34 \times 10^{-4}$ ,  $L_{cv} = 1.72$  km,  $L_{ch} = 32.9$  km. The vertical spatial spacing = 0.1 km, transverse spacing = 0.1 km, and line-of-sight spacing = 15.7 km. The curves show log-log plots of *PSD*'s measured in  $(\delta T / \text{Temperature})^2$  and wavenumber measured in  $\text{km}^{-1}$ . The vertical autoregressive *PSD* for the simulation was computed by calculating a 6 coefficient forward and backward

Memo

19. PSD estimates of the horizontally scanned simulated atmosphere from Autoregressive analysis.
20. Two-Dimensional image temperature structure scene from 3-D simulation. Artificial temperature sensor located at 85 km.

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autoregressive model of the vertically simulated data from layers extending from 50.0 km to 50.6 km in the forward direction and layers extending from 51.2 km to 50.6 km in the backward direction. Note that the "transverse" direction is defined as the horizontal perpendicular to the "line-of-sight" direction. The transverse and line-of-sight PSD's represent the 1-D component of the 2-D horizontal PSD having a high frequency horizontal spectral slope = -8/3. Their autoregressive PSD's result from computing a 10 coefficient autoregressive model of the transverse and line-of-sight simulated data in the layer at 50.6 km. The transverse Nyquist frequency is approximately  $1/(2 \times 0.1) = 5 \text{ km}^{-1}$  and the line-of-sight Nyquist frequency is approximately  $1/(2 \times 15.7) = 0.032 \text{ km}^{-1}$ .

7. One dimensional periodograms of the first four samples of the line-of-sight simulated data in the layer at 50.6 km.
8. Same as figure 6 except altitude = 119.3 km,  $\sigma^2 = 0.0277$ ,  $L_{cv} = 2.42 \text{ km}$ , and  $L_{ch} = 49.1 \text{ km}$ . The transverse spacing is 0.101 km and LOS spacing is 15.9 km.
9. Histogram representing the probability distribution function of the simulated data at 50.6 km. Solid line is the theoretical Gaussian pdf. The variance of the data is  $8.35 \times 10^{-4}$ .
10. Cumulative distribution function of the simulated data at 50.6 km compared to the theoretical curve.
11. Sample page from the database explanation file.
12. Alias branches of estimated "theoretical" LOS PSD.
13. "Theoretical" transverse PSD versus a 512 point PSD "corrected" for truncation of the autocorrelation function. The plot has the same input parameters previously given for 50.6 km altitude. The one-dimensional high frequency spectral slope is  $(S) = -5/3$ ,  $\sigma^2 = 8.34 \times 10^{-4}$ ,  $L_{ch} = 32.9 \text{ km}$ , and transverse spacing = 0.1 km.
14. Approximation correction for rectangular window discrete Fourier Transform digital sinc function.
15. Viewing geometry of an imaginary temperature sensor platform located at an altitude of 85 km.
16. Integrated temperature structure along selected pixel rows comprising zenith look angles from the minimum of 94.60 to the maximum of 960
17. Integrated temperature structure along selected pixel columns comprising horizontal look angles from -.01870 to +.01870.
18. Fourier periodograms of the horizontally scanned simulated atmosphere for the same look angles of Figure 16.

# **GOAL - Create Synthetic 3-D Atmospheric Temperature Structure Database**

- Consistent with specified PSD's, statistics, and correlation lengths
- Minimizes computational burden and storage requirements
- Applicable to Radiance Structure Models



# Stepping Stones

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- 1-D Model
  - An Autoregressive Model for Smooth Geophysical Power Spectra with Known Autocorrelation Function, PL-TR-93-2016
- 2-D Model
  - Atmospheric Structure Simulation: An ARMA Model for Smooth Isotropic Two-Dimensional Power Spectra, PL-TR-93-2224

# Linear Difference Equation

---

$$x(n) = - \sum_{k=1}^p a(k)x(n-k) + \sum_{k=0}^q b(k)\epsilon(n-k)$$



# Power Spectra Model



$$P_{ARMA}(f) = T \rho_w \left| \frac{B(f)}{A(f)} \right|^2$$

$$A(f) = 1 + \sum_{k=1}^p a(k) \exp(-2\pi ifkT)$$

$$B(f) = 1 + \sum_{k=0}^q b(k) \exp(-2\pi ifkT)$$

$$x(n) = - \sum_{k=1}^p a(k) x(n-k) + \varepsilon(n)$$

$$P_{AR}(f) = \frac{T \rho_w}{|A(f)|^2} = T \sum_{k=-\infty}^{\infty} r_{xx}(k) \exp(-2\pi ifkT)$$

# Yule Walker Equations

$$r_{xx}(m) = \begin{cases} -\sum_{k=1}^p a(k)r_{xx}(m-k) & \text{for } m > 0 \\ -\sum_{\substack{k=1 \\ *}}^p a(k)r_{xx}(-k) + \rho_w & \text{for } m = 0 \\ r_{xx}(-m) & \text{for } m < 0 \end{cases}$$

$$\begin{pmatrix} r_{xx}(0) & r_{xx}(-1) & \cdots & r_{xx}(-p) \\ r_{xx}(1) & r_{xx}(0) & \cdots & r_{xx}(-p+1) \\ \vdots & \vdots & \ddots & \vdots \\ r_{xx}(p) & r_{xx}(p-1) & \cdots & r_{xx}(0) \end{pmatrix} \begin{pmatrix} 1 \\ a(1) \\ \vdots \\ a(p) \end{pmatrix} = \begin{pmatrix} \rho_w \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

# Levinson Recursion Algorithm

$$a_k[k] = - \frac{r_{xx}[k] + \sum_{\ell=1}^{k-1} a_{k-1}[\ell] r_{xx}[k-\ell]}{\rho_{k-1}}$$

$$a_k[i] = a_{k-1}[i] + a_k[k] a_{k-1}^*[k-i] \quad i = 1, 2, \dots, k-1$$
$$\rho_k = \left(1 - |a_k[k]|^2\right) \rho_{k-1}$$

with ,

$$a_1[1] = - \frac{r_{xx}[1]}{r_{xx}[0]}$$

$$\rho_1 = \left(1 - |a_1[1]|^2\right) r_{xx}[0]$$

# PSD of Simulated Series

$$\text{PSD}(f) = \frac{2\sigma_c^2 \Delta x}{\left| 1 + \sum_{i=1}^{NN} b_i e^{j2\pi f \Delta x} \right|^2}$$

Minimize ERR,

$$\text{ERR} = \left( \sum_{J=NN+1}^M \left( Y(J) - \sum_{i=1}^{NN} b_i Y(J-i) \right)^2 \right) + \left( \sum_{J=1}^{M-NN} \left( Y(J) - \sum_{i=1}^{NN} b_i Y(J+i) \right)^2 \right)$$

$$\sigma_c^2 = \frac{\text{ERR}}{2(M-NN)}$$

## **PSD and ACF Models**

---

$$\text{PSD}(k) = \frac{\sigma^2 a^{2v} \Gamma\left(v + \frac{1}{2}\right)}{\sqrt{\pi} \Gamma(v) \left(a^2 + k^2\right)^{v + \frac{1}{2}}}$$
$$\text{ACF}(x) = \frac{\sigma^2 2^{(1-v)} (2\pi a x)^v K_v(2\pi a x)}{\Gamma(v)}$$

## Coherence Length Parameter

$$L_c = \frac{\Gamma\left(\nu + \frac{1}{2}\right)}{2\sqrt{\pi}\Gamma(\nu)a}$$

## 2-D PSD

$$PSD_{theor}(f_x, f_y) = \frac{\sigma^2 v a^{2\nu}}{\pi(a^2 + f_x^2 + f_y^2)^{\nu+1}}$$

$$S(x, y) = FFT^{-1} \left( \sqrt{\frac{PSD_{theor}(f_x, f_y)}{\Delta x \Delta y}} \times FFT(\tilde{G}(\mathcal{E}_x, \mathcal{E}_y)) \right)$$

In practice, the PSD is adjusted to accord with sampling and convolution theory. For low frequency resolution along the transverse direction, the PSD is adjusted to account for rectangular windowing of deccretized samples. This is the "Sinc" function effect.

For low Nyquist frequency along the LOS direction, the PSD is adjusted to account for an aliasing effect.

# Transverse correction for large resolution frequency - rectangular window Sinc sampling problem

$f_y \equiv \text{Los direction}$

$f_x \equiv \text{Transverse direction}$

Where,  $A^2(f_x, f_y) = PSD(f_x, f_y) / \Delta x \Delta y$

Modify  $A(0, f_y)$  to  $A_1(0, f_y)$  by:

$$A_1(0, f_y) = g A(0, f_y) + (1 - g) A(1, f_y)$$

such that

$$\sigma^2 = \sum_{f_x} \sum_{f_y} A_1^2(f_x, f_y)$$

# LOS correction for small Nyquist frequency

---

$f_y \equiv$  Los direction

$f_x \equiv$  Transverse direction

For  $0 < f_y < f_{Ny}$  Measured PSD at  $f_y$  is:

$$\begin{aligned} PSD_m(f_x, f_y) = & PSD(f_x, f_y) + PSD(f_x, 2f_{Ny} - f_y) \\ & + PSD(f_x, 2f_{Ny} + f_y) + PSD(f_x, 4f_{Ny} - f_y) \\ & + PSD(f_x, 4f_{Ny} + f_y) + \dots \end{aligned}$$

# Conclusions

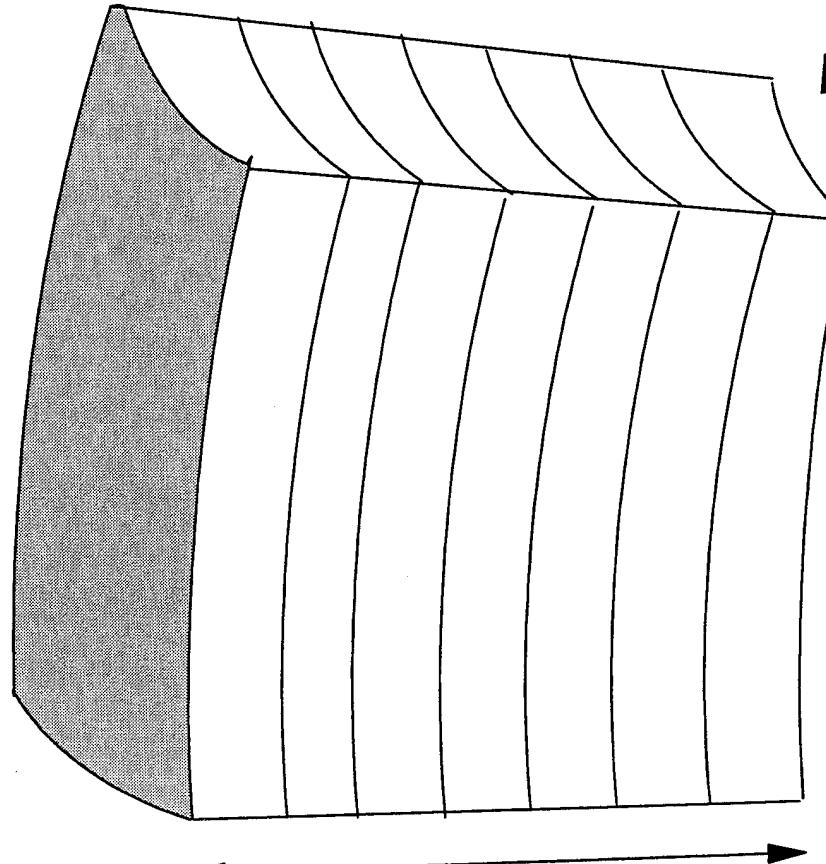
- Autoregressive synthesis (6 coef.) accurately models 1-D vertical geophysical PSD's
- Fast Fourier Transform synthesis accurately models 2-D horizontal geophysical PSD's
- Accounting for discretized samples, hybrid method preserves slope, coherence length, variance, and pdf (also LOS)
- Hybrid system "builds in" non-stationarity
- Generation of entire 3-D database in 2.5 Hrs.

# Database Specifications

Direction	Npts	$\Delta x$ (km)	$N\Delta x$ (km)	freq. res. $1/N\Delta x$ (cy/km)	Nyquist freq $1/2\Delta x$ (cy/km)
Vertical (50-120 km)	700	.1	70	---	---
Transverse	512	.1	51.2	.0195 (HIGH)	5
LOS	192	15.7	3014.	.00033	.0318 (LOW)

# Database Geometry

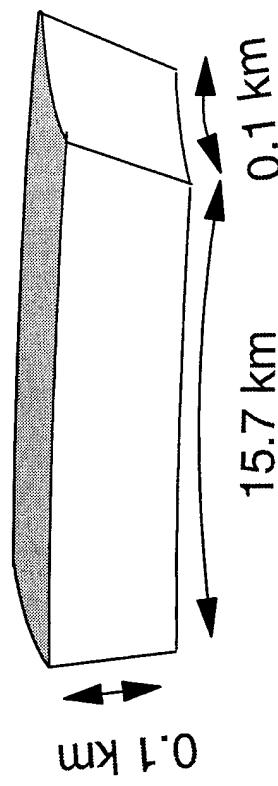
Line-of-Sight Direction



3014 Km

1.2 Km  
Transverse  
Direction

70 Km



15.7 Km

0.1 Km



3 /

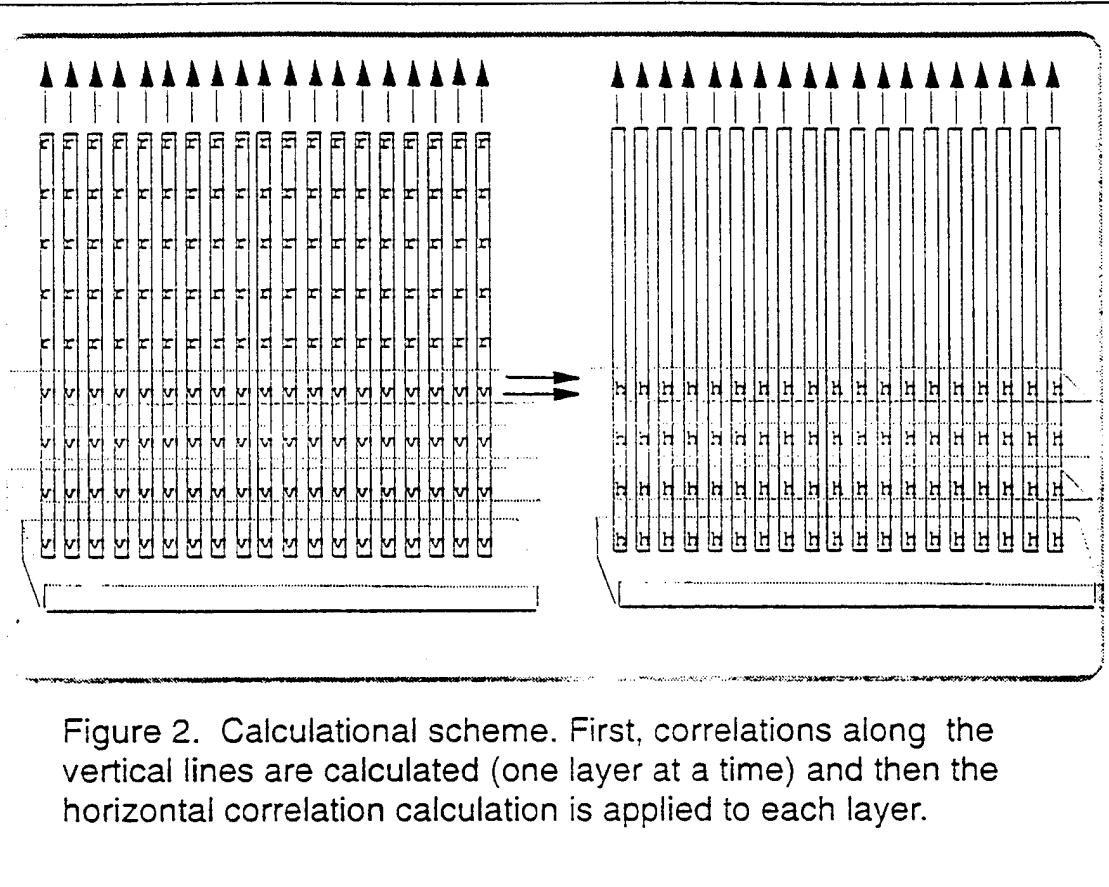
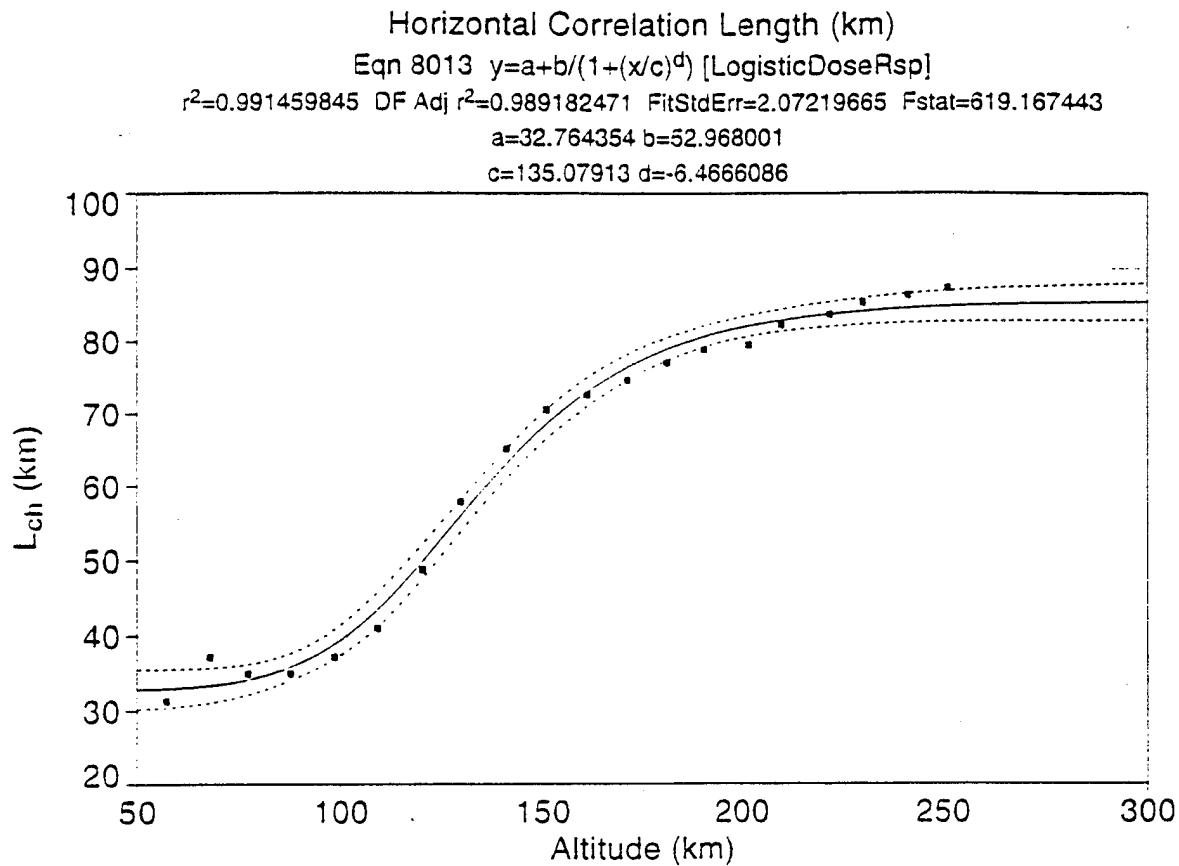


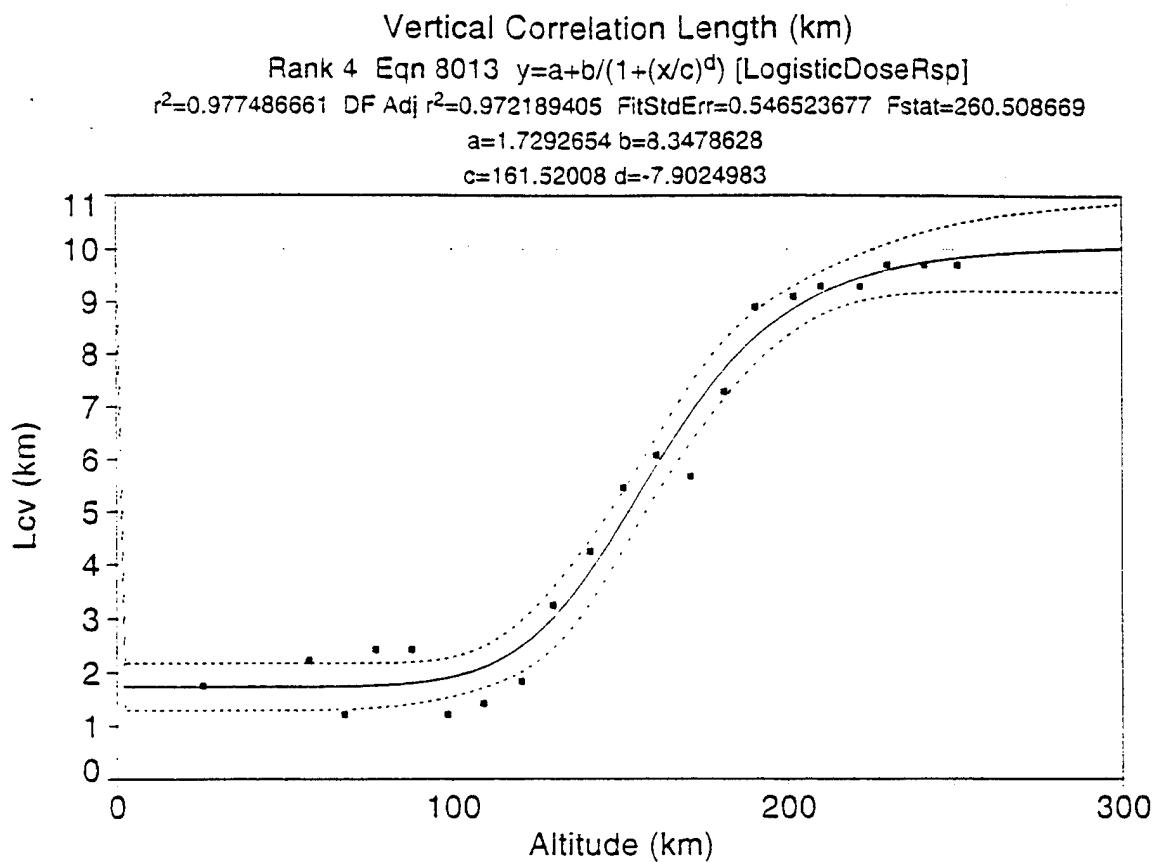
Figure 2. Calculational scheme. First, correlations along the vertical lines are calculated (one layer at a time) and then the horizontal correlation calculation is applied to each layer.



Rank 18 Eqn 8013  $y=a+b/(1+(x/c)^d)$  [LogisticDoseRsp]

$r^2$	Coef Det	DF	Adj $r^2$	Fit Std Err	F-value
0.9914598452		0.9891824705		2.0721966466	619.16744310

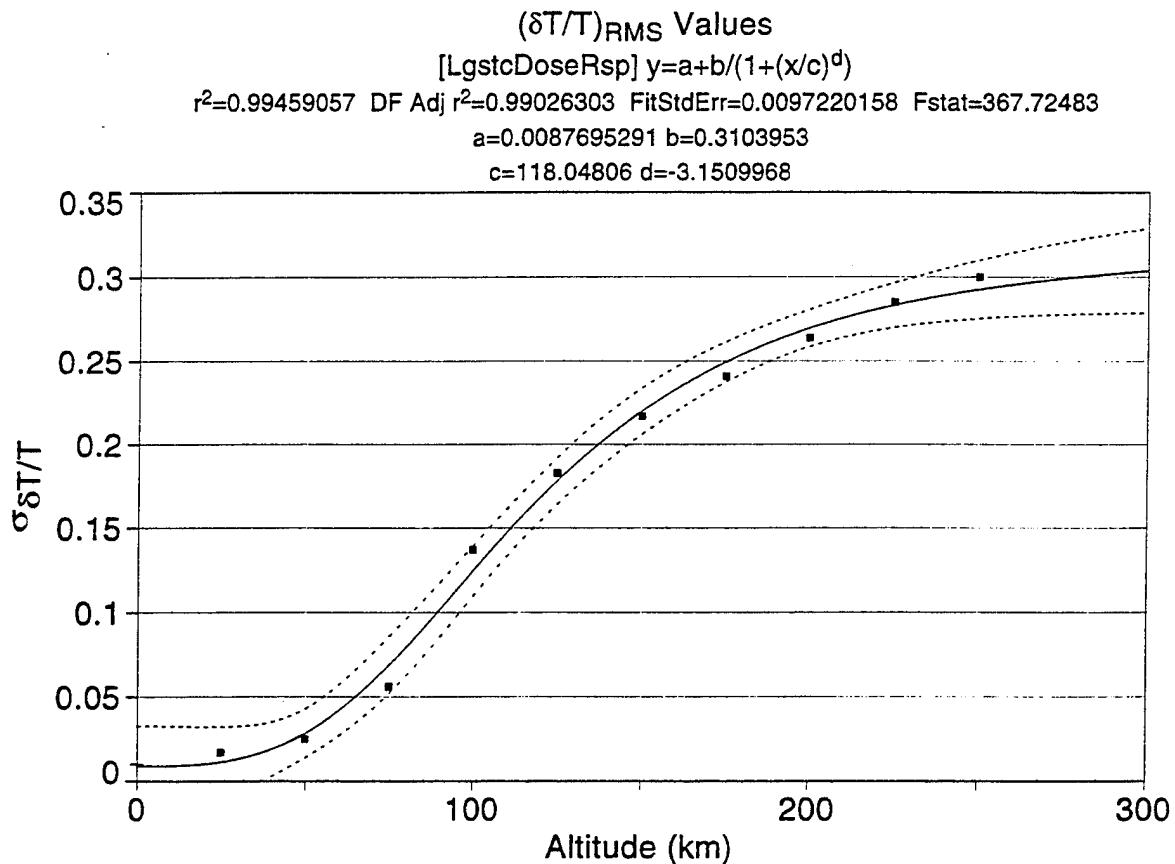
Parm	Value	Std Error	t-value	95% Confidence Limits	
a	32.76435426	1.295628218	25.28839199	30.01210311	35.51660541
b	52.96800100	2.144297606	24.70179552	48.41295545	57.52304655
c	135.0791315	2.234742679	60.44504933	130.3319571	139.8263059
d	-6.46660858	0.680074818	-9.50867230	-7.91126428	-5.02195287



Rank 4 Eqn 8013  $y=a+b/(1+(x/c)^d)$  [LogisticDoseRsp]

$r^2$	Coef Det	DF	Adj $r^2$	Fit Std Err	F-value
0.9774866610		0.9721894048		0.5465236769	260.50866885

Parm	Value	Std Error	t-value	95% Confidence Limits
a	1.729265412	0.210585414	8.211705540	1.286422835 2.172107988
b	8.347862811	0.536310568	15.56535207	7.220048927 9.475676694
c	161.5200848	3.853308016	41.91725244	153.4169175 169.6232522
d	-7.90249825	1.339177504	-5.90100881	-10.7186706 -5.08632592

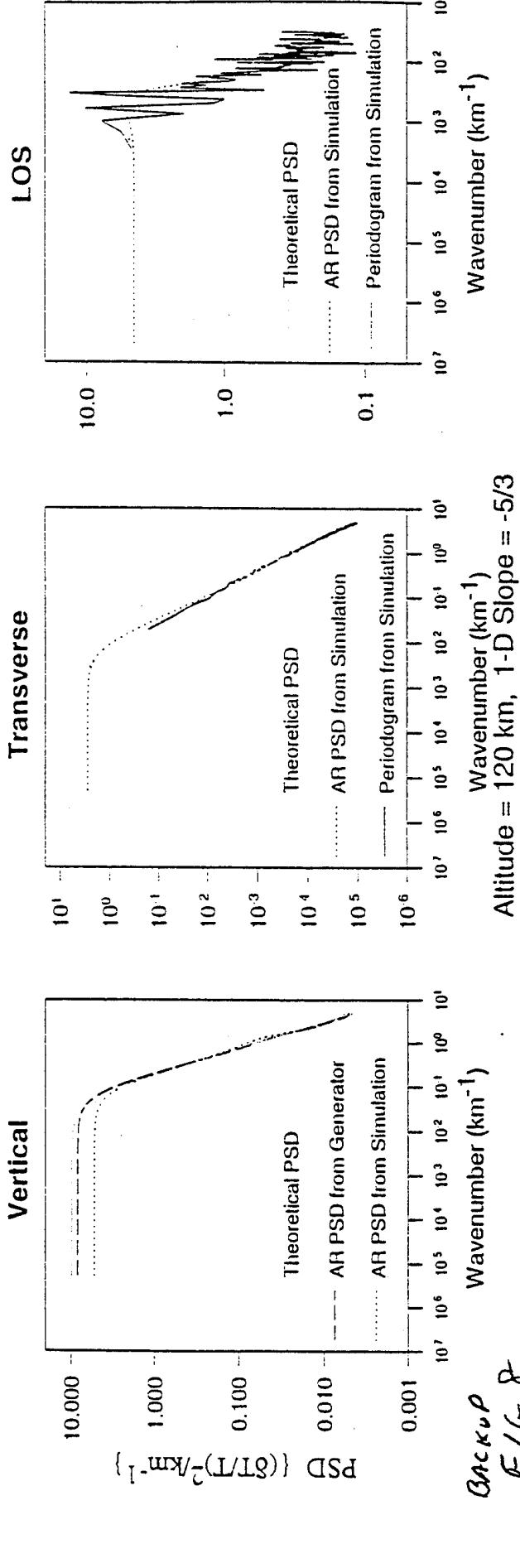
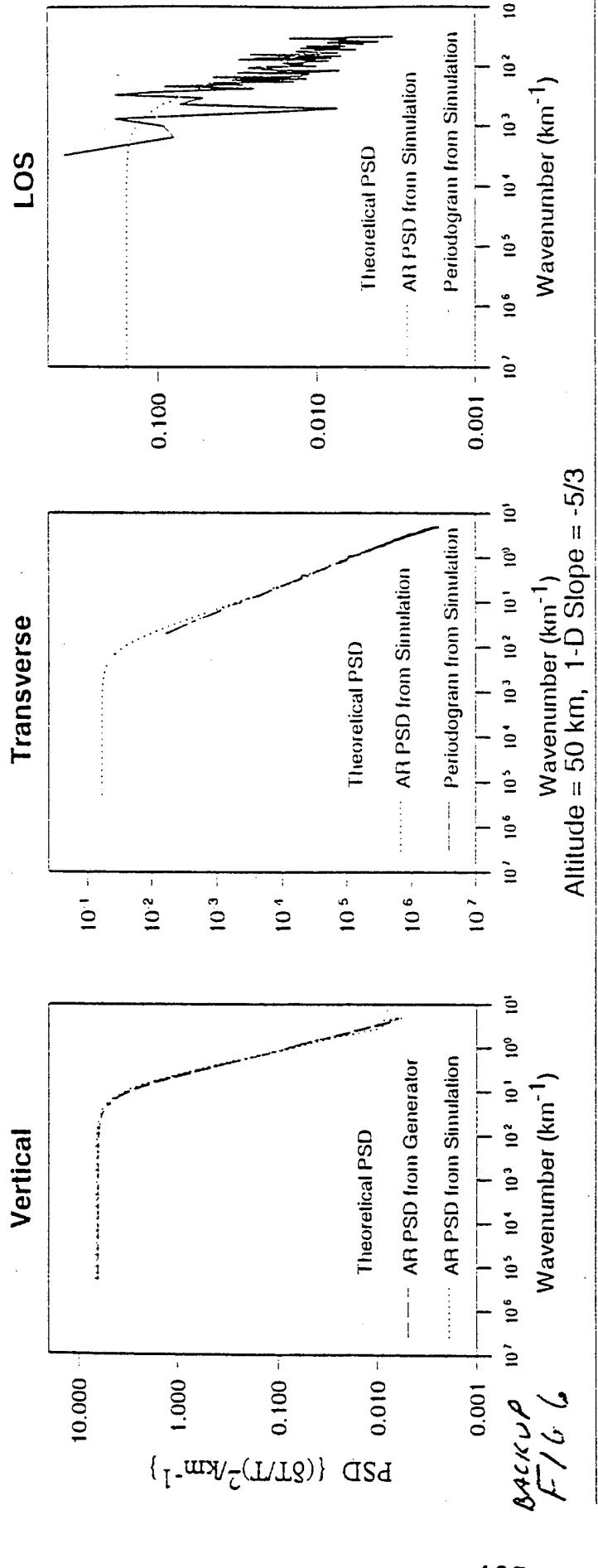


Rank 931 Eqn 8013 [LgscDoseRsp]  $y=a+b/(1+(x/c)^d)$

$r^2$	Coef Det	DF Adj $r^2$	Fit Std Err	F-value
0.9945905715		0.9902630287	0.0097220158	367.72482563

Parm	Value	Std Error	t-value	95% Confidence Limits
a	0.008769529	0.009675816	0.906334825	-0.01500493 0.032543990
b	0.310395297	0.024196036	12.82835344	0.250943187 0.369847408
c	118.0480550	5.745293881	20.54691326	103.9312859 132.1648241
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 MODIFY ZERO FREQ TO GIVE CORRECT VARIANCE GREAT CIRCLE APPROXIMATION FOR HOURS 6.370E-03  
 ROTATION NUMBER SEED= 12345 QLITUDE NUMBER 7 = 5.09E-01 SHORE IV= 1.67E-00 THIS MEANS KUVI= 3.33E-01 SHOREIV= 1.00E-01  
 IW=16.90E-02 LCV=1.72E-00 NUMBER OF ROTATION SAMPLES=99304 NUMBER OF PREDICTOR COEFFICIENTS V=6 H=10  
 NUMBER OF ITERATIONS=51 THIS IS ONE SHEET OF 512 PERIODICAR VALUES BY 192 L.O.S. VALUES SHORE\*2 WILL BE SET TO 0.34E-04  
 PERIODICAR SPACING=1.00E-01 SPACING L.O.S.=1.57E-01 QLIE=3.62E-03 QLIE=3.29E-01 SLOPE10H=2.67E+00 THIS MEANS NUMBER 3.33E-01  
 INTEGRAL OF PSD= 0.99E-04

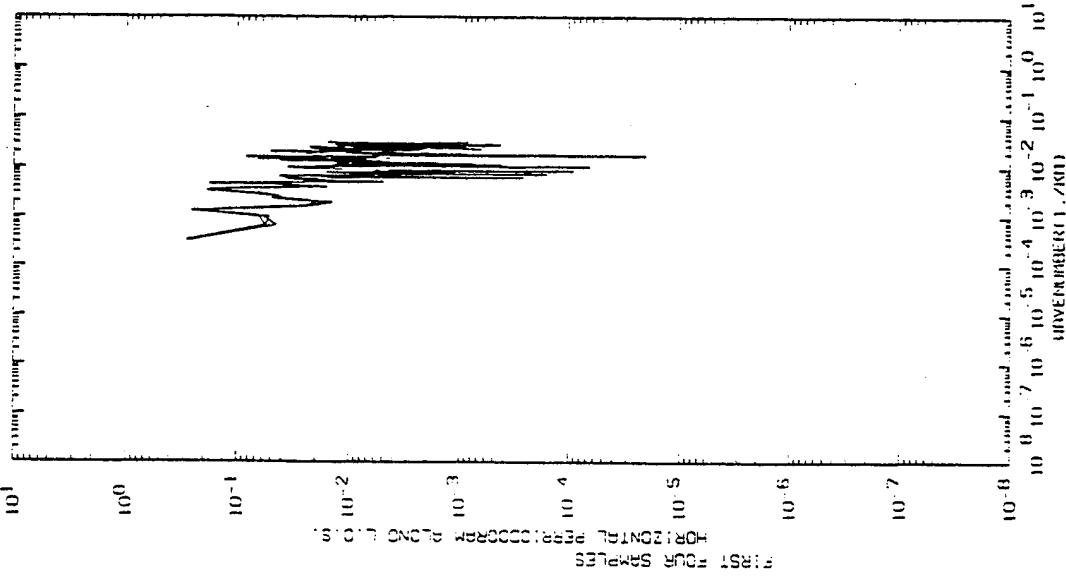
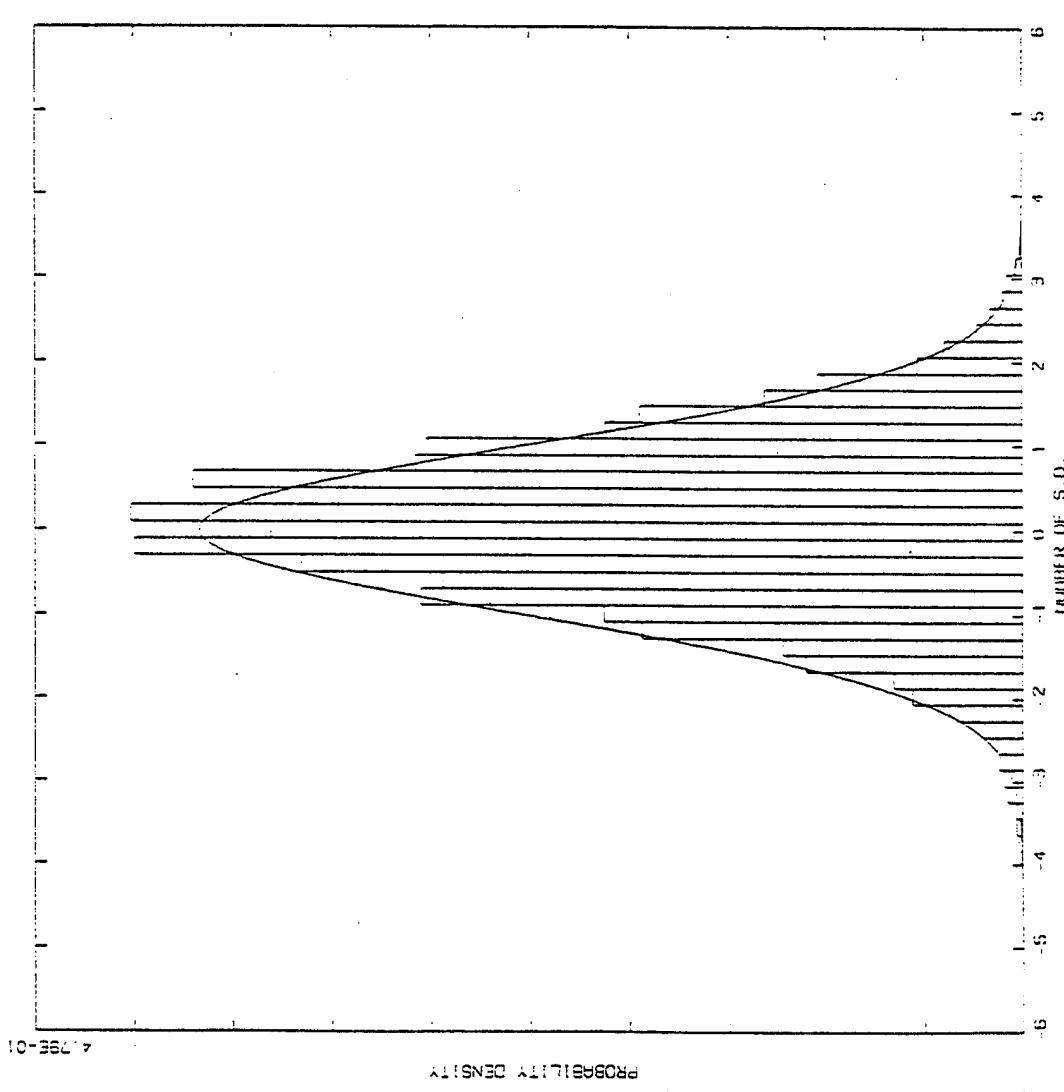


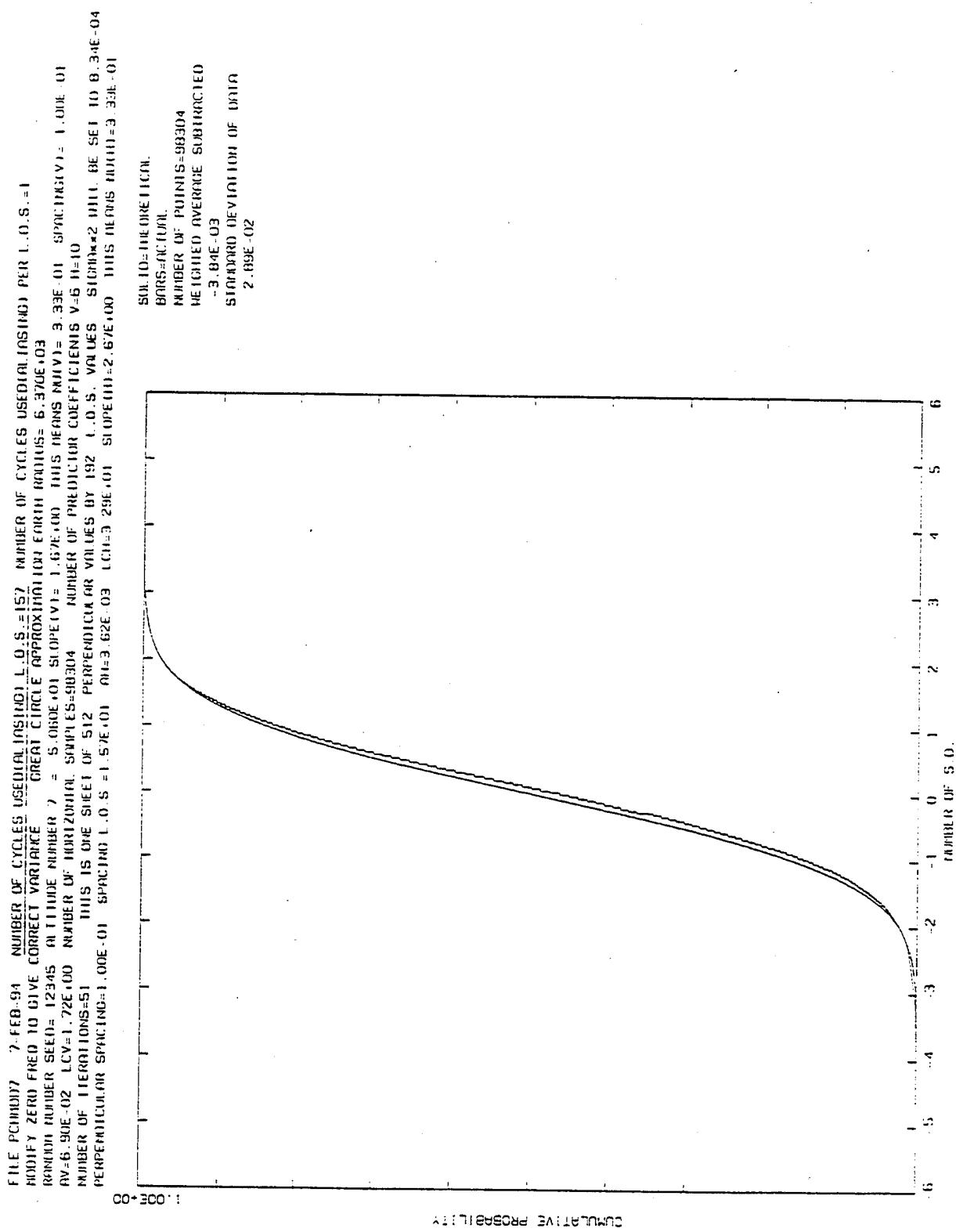
FIG 7

FILE PCINH07 7-FEB-94 NUMBER OF CYCLES USED ON LASTING L.O.S.=157 NUMBER OF CYCLES USED ON LOSING PER L.O.S.=1  
 MODIFY ZERO FREQ TO GIVE CORRECT VARIANCE GREAT CIRCLE APPROXIMATION EARTH RADIUS= 6.370E+03  
 RANDOM NUMBER SEED= 12345 AL TIME NUMBER ? = 5.00E+01 SLOPE(V)= 1.67E+00 THIS MEANS MU(V)= 3.33E-01 SLOPE(MG(V))= 1.00E-01  
 $\Delta V=6.90E-02$  LCV=1.72E+00 NUMBER OF HORIZON POINTS=90304 NUMBER OF PREDICTOR COEFFICIENTS V=6  $H=10$   
 NUMBER OF ITERATIONS=51 THIS IS ONE SHEET OF 512 PREDICTOR COEFFICIENTS FOR VALUES BY 152 L.O.S. VAMES SIGHTS=2000.00 THE SEI TO 0.34E-04  
 PERPENDICULAR SPACING=1.00E-01 SPACING L.O.S.=1.57E+01  $\Delta H=3.62E-03$   $LCH=3.29E+01$  SLOPE(H)=2.67E+00 THIS MEANS MU(H)=3.33E-01

SOL 10=THEORETICAL  
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 NUMBER OF POINTS=90304

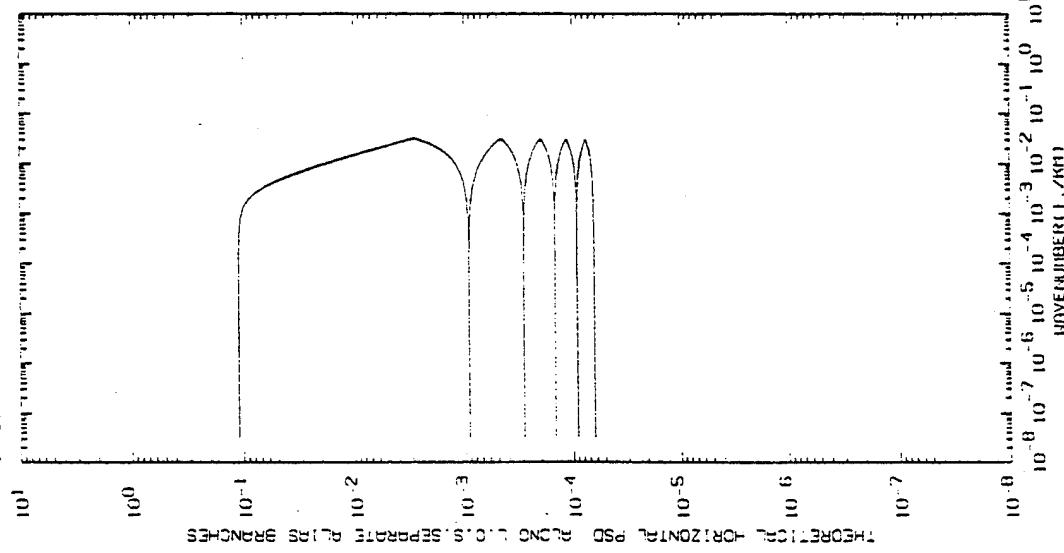
WEIGHTED AVERAGE STANDARD DEVIATION OF DATA  
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 STANDARD DEVIATION OF DATA  
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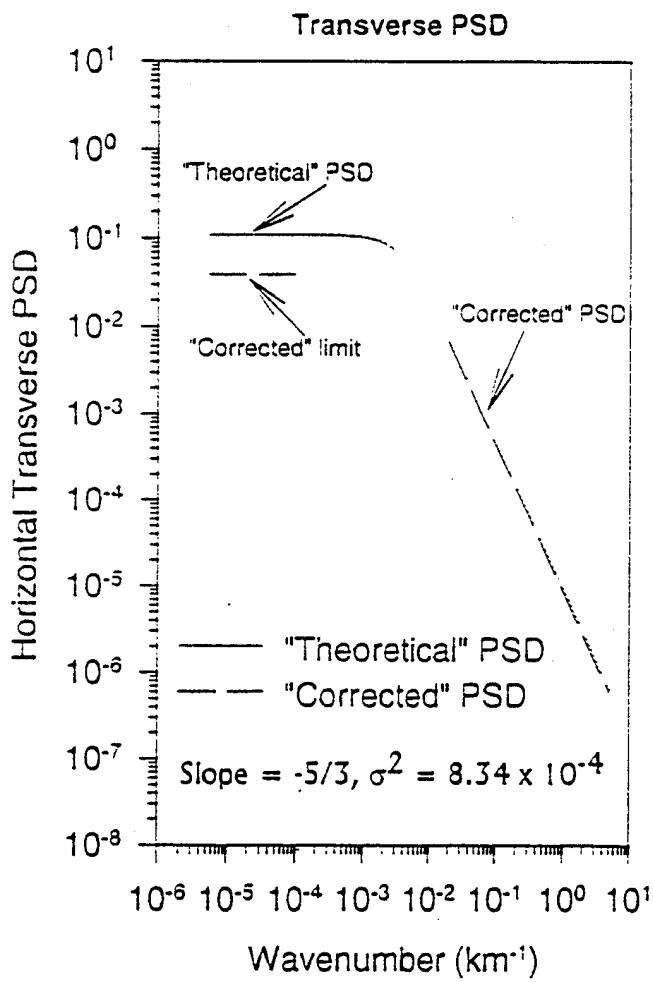


POINTS FROM SHEET OF HORIZONTAL DATA

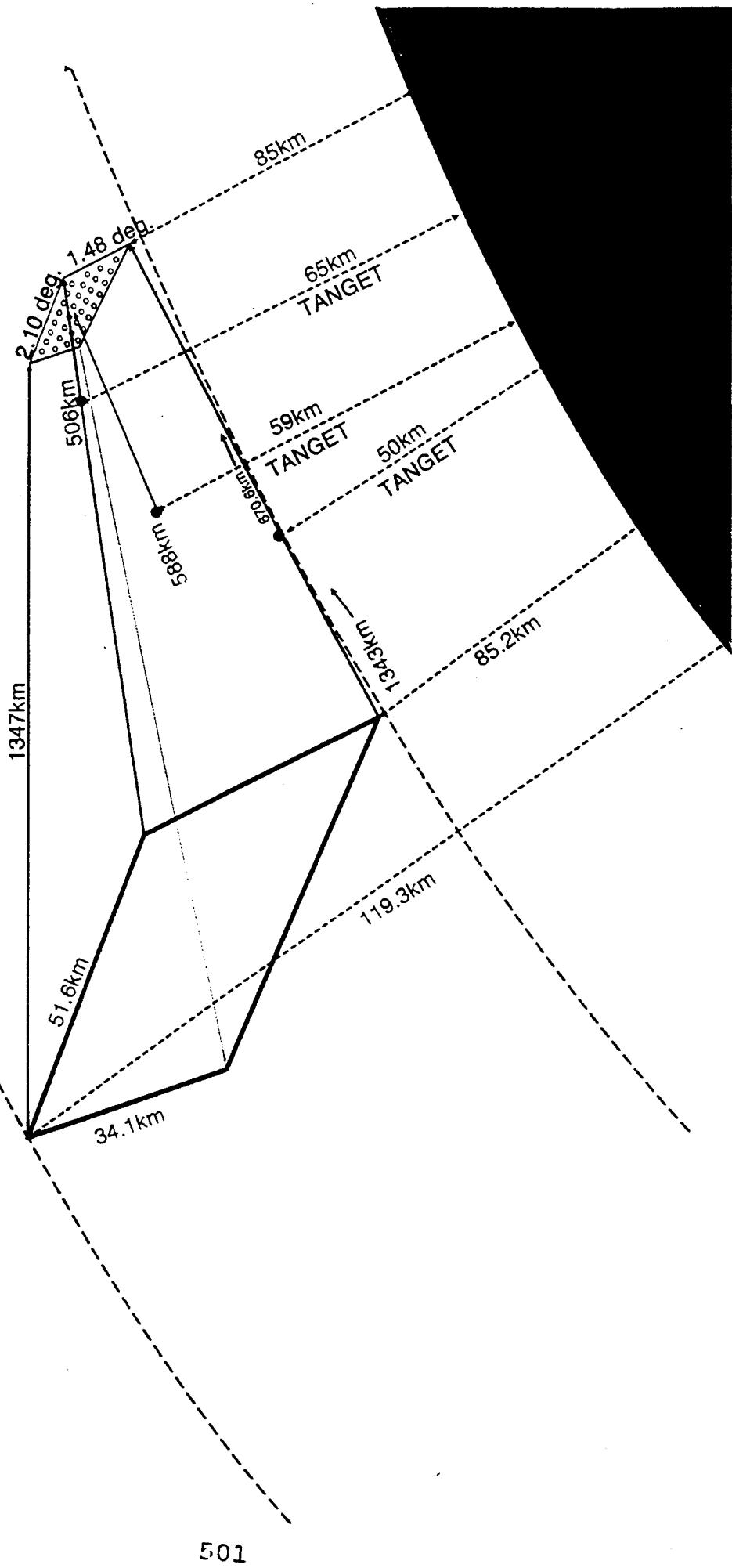
FILE PC1H006 7-FEB-94 GREAT CIRCLE APPROXIMATION EARTH RADIUS= 6.370E-09  
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 INTERIOR OF PSO= 0.29E-04 THIS IS STEP 1 NUMBER 7 BIGS PSO NUMBER. TO GIVE CORRECT WORKING



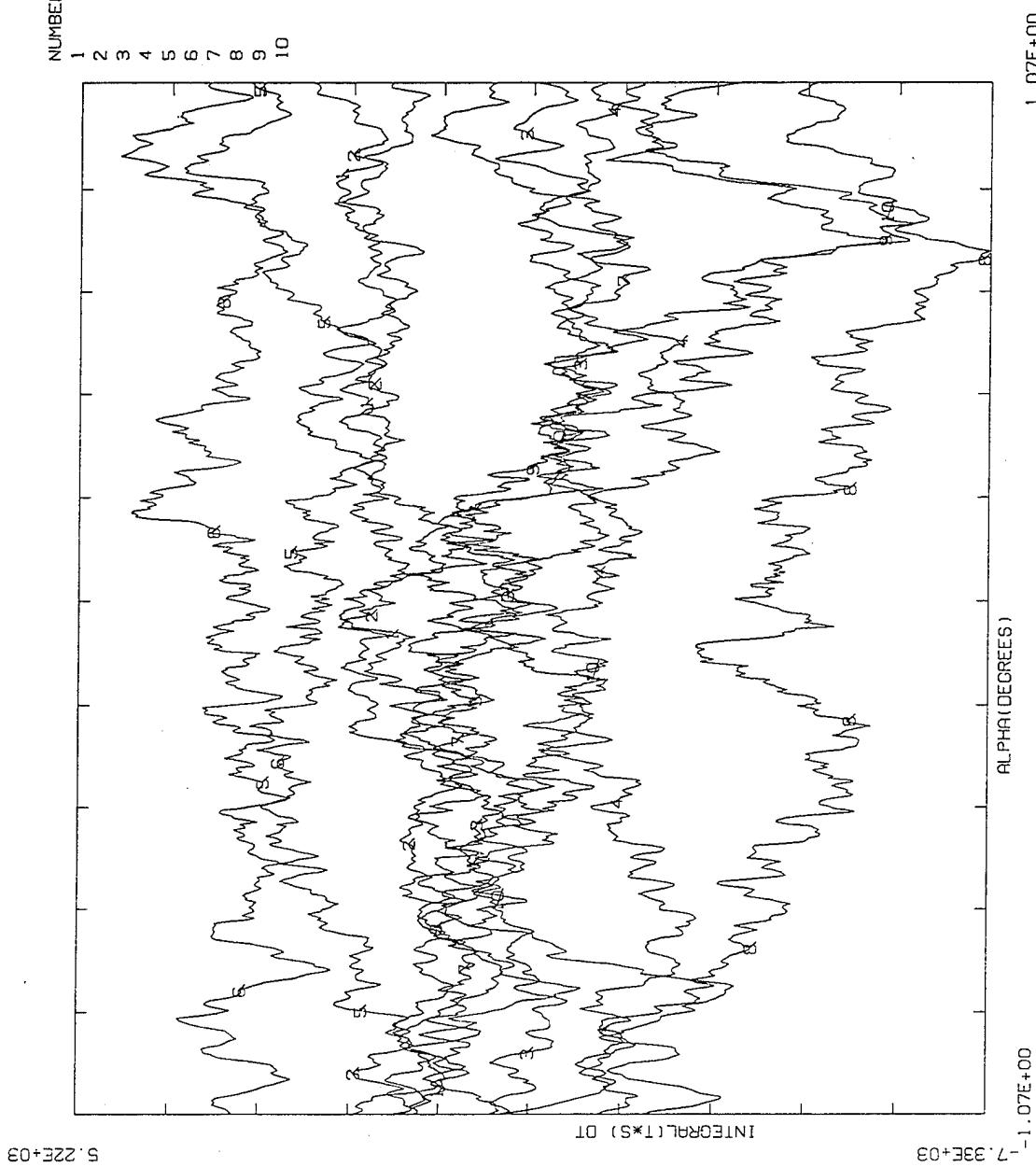
Backup F16 12



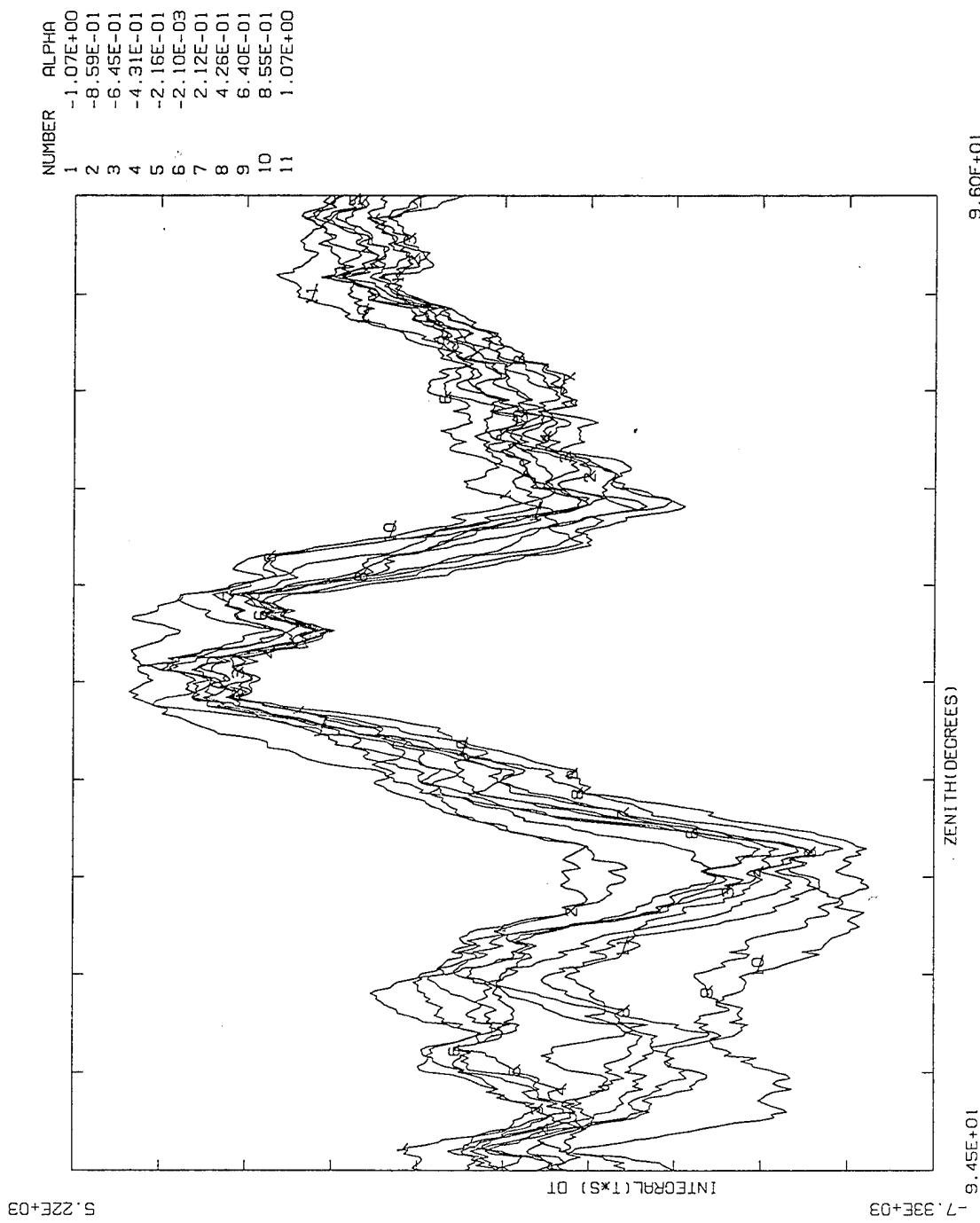
BACKUP F-16 13



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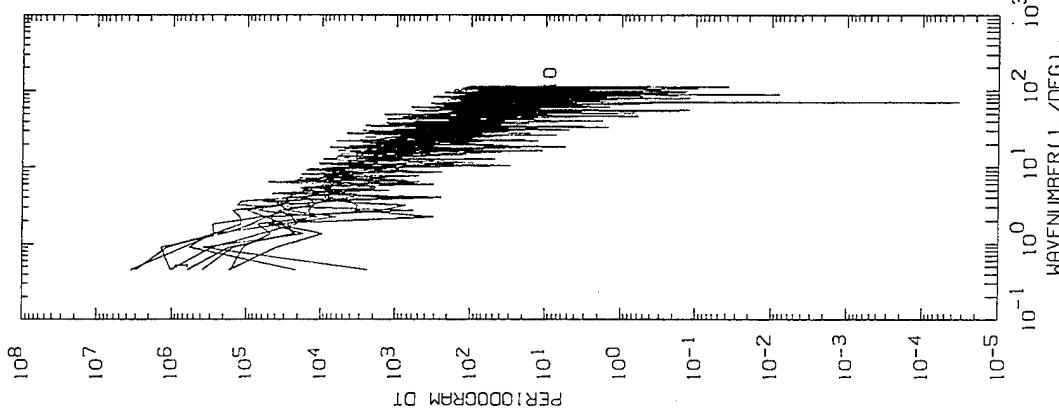


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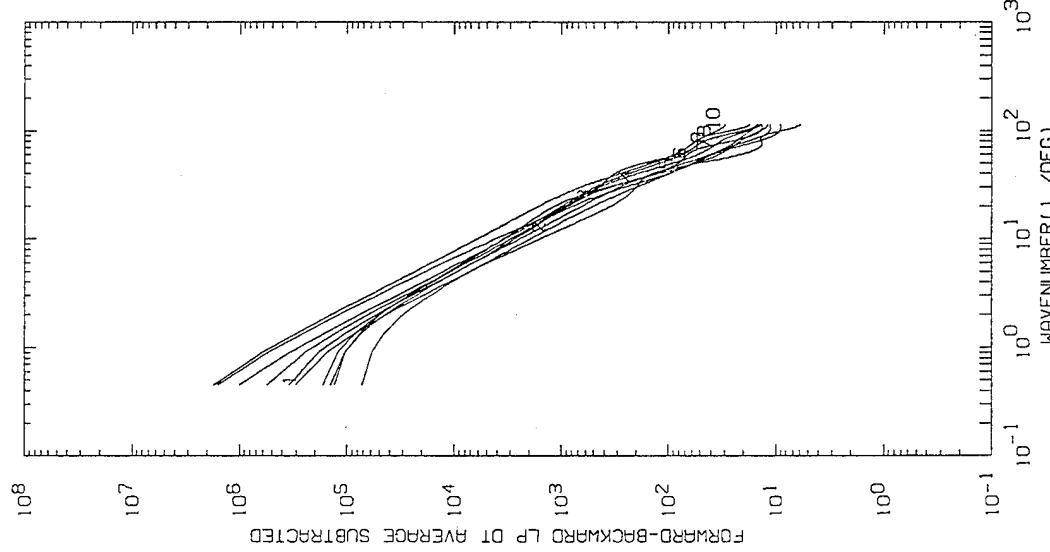
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5	9.54E+01
6	9.52E+01
7	9.51E+01
8	9.49E+01
9	9.48E+01
10	9.46E+01



VALUES FOR PSD

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 MAXIMUM ANGLE L.O.S. USED= 1.19E+01 DEGREES NUMBER OF ZENITH VALUES CALCULATED=350 CENTER ZENITH VALUE= 9.52E+01 DEGREES  
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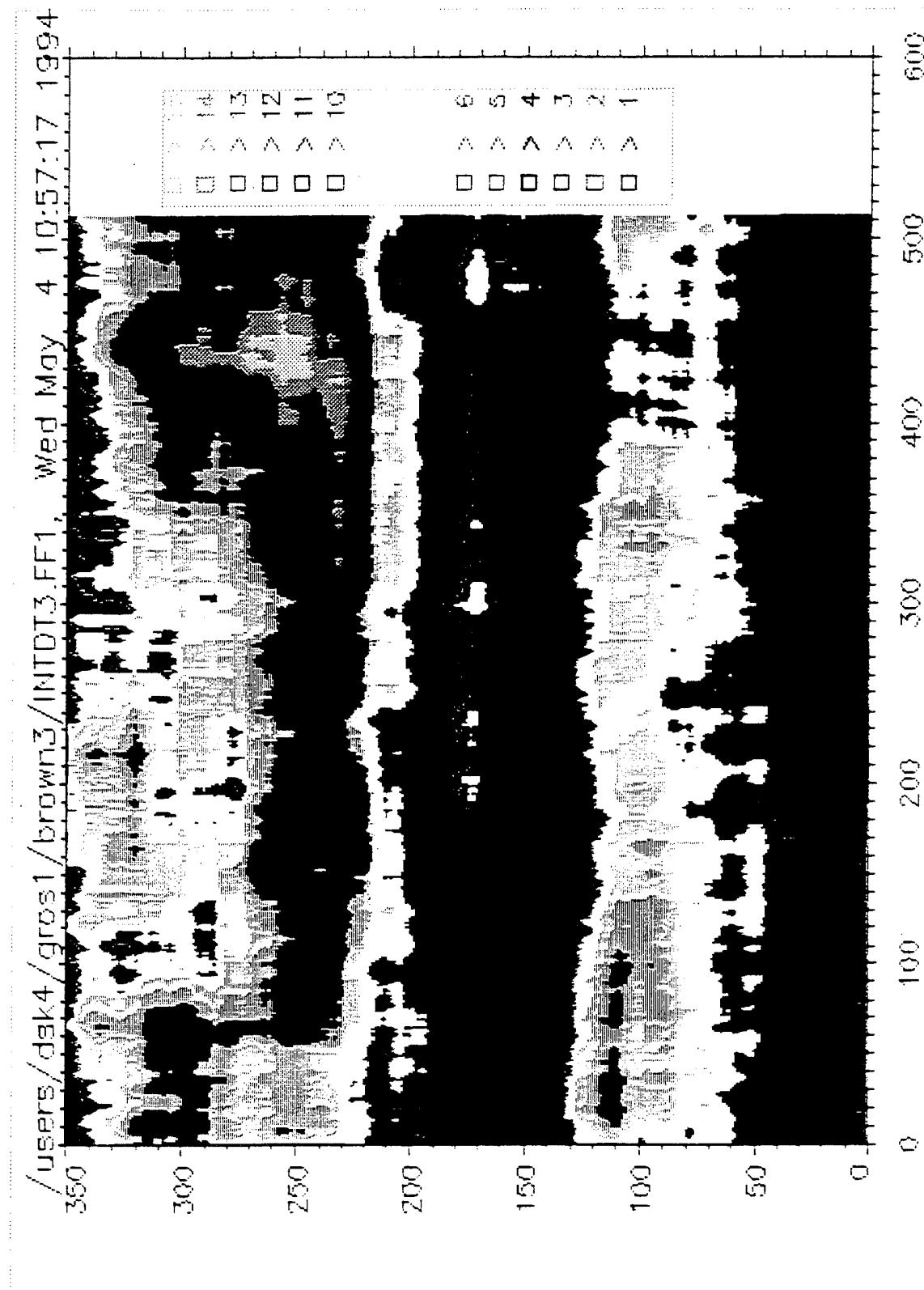
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7	9.51E+01
8	9.49E+01
9	9.48E+01
10	9.46E+01



NUMBER OF LP COEFFICIENTS 6  
 VALUES FOR PSD

13 APR 1994 10:00 / 9

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# Plane Wave Scintillation in an Onion Skin Model

Robert R. Beland  
Phillips Laboratory

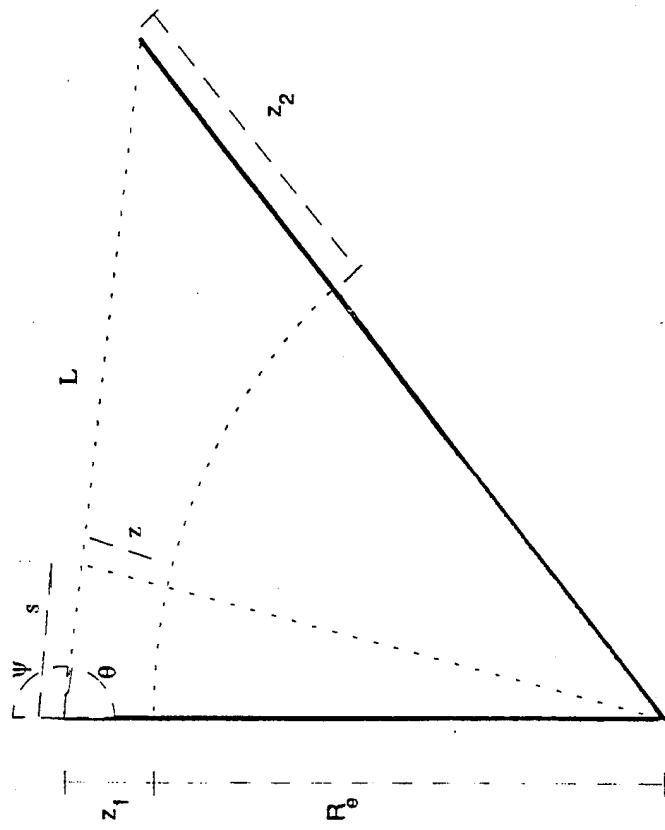
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Annual Review Conference on Atmospheric Transmission Models  
**7-8 June 1994**

## Objectives

- include horizontal variability of atmospheric turbulence through long near horizontal paths
- emphasize application to aircraft-based platforms
- derive analytic expressions for Rytov theory scintillation with onion skin model
- compare predictions with existing approaches
- investigate effects of aperture averaging and inner scale
- compare Rytov/onion skin predictions with data

## Definition of Onion Skin Geometry



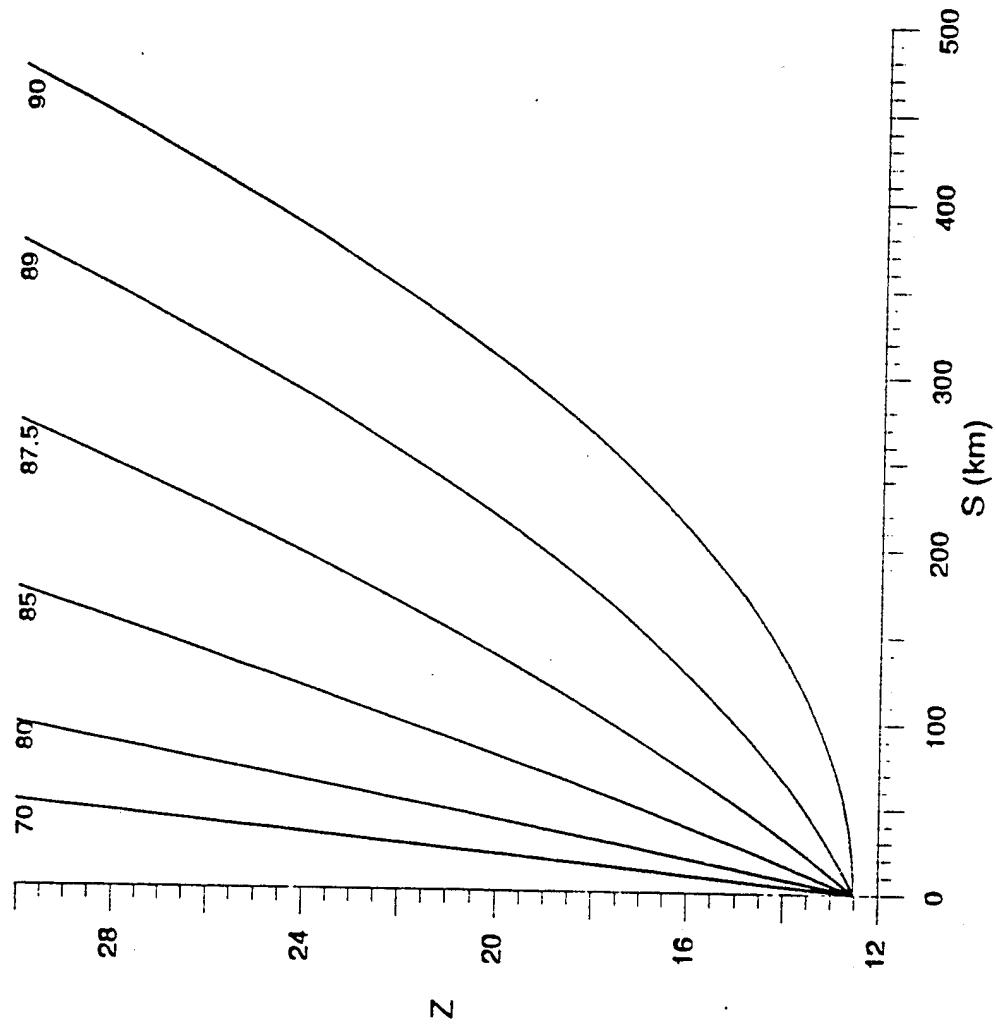
$$\cos(\psi) = \frac{R_2^2 - L^2 - R_1^2}{2R_1L}$$

$$s = f(z, \psi)$$

$$= \sqrt{R^2 - R_1^2 \sin^2(\psi) - R_1 \cos(\psi)}$$

$$= \sqrt{(R_e + z)^2 - (R_e + z_1)^2 \sin^2(\psi) - (R_e + z_1) \cos(\psi)}$$

Altitude of the propagation path for a 12.5 km observer for various zenith angles



## Onion Skin Model and the Log Amplitude Variance

The Rytov solution for a plane wave originating at L and observed at s=0 (point detector)

$$\sigma_{\chi}^2 = 4\pi^2 k^2 \int_0^L ds \int_0^\infty dK K \Phi_n(K, s) \sin^2 \left( \frac{K^2 s}{2k} \right)$$

$$\text{For the Kolmogorov spectrum: } \quad \sigma_{\chi}^2 = 0.56k^{7/6} \int_0^L C_n^2(s) s^{5/6} ds$$

**Flat Earth Model:** Assume that  $C_n^2$  is only a function of altitude. Explicitly, assume:

$$1) \quad s = (z - z_1) \sec(\psi)$$

$$2) \quad C_n^2(s) = C_n^2(z)$$

Then

$$\sigma_{\chi}^2 = 0.56k^{7/6} \{ \sec(\psi) \}^{14/6} \int_{z_1}^{z_2} C_n^2(z) (z - z_1)^{5/6} dz$$

## Onion Skin Model

Assume  $C_n^2$  is a function only of altitude, but include the earth's curvature. The atmosphere is treated as concentric shells or layers. Explicitly, assume:

$$1) \quad s = f(z, \psi)$$

$$2) \quad C_n^2(s) = C_n^2(z)$$

Then

$$\sigma_\chi^2 = 0.56k \int_{z_1}^{z_2} C_n^2(z) [f(z, \psi)]^2 f'(z, \psi) dz$$

where

$$s = f(z, \psi) = \sqrt{(R_e + z)^2 - (R_e + z_1)^2 \sin^2(\psi)} - (R_e + z_1) \cos(\psi)$$

$$f'(z, \psi) = \frac{ds}{dz} = \frac{(R_e + z)}{\sqrt{(R_e + z)^2 - (R_e + z_1)^2 \sin^2(\psi)}}$$

Define the altitude weighting function,  $W(z, \psi)$

$$\sigma_x^2 = \int_{z_1}^{z_2} C_n^2(z) W(z, \psi) dz$$

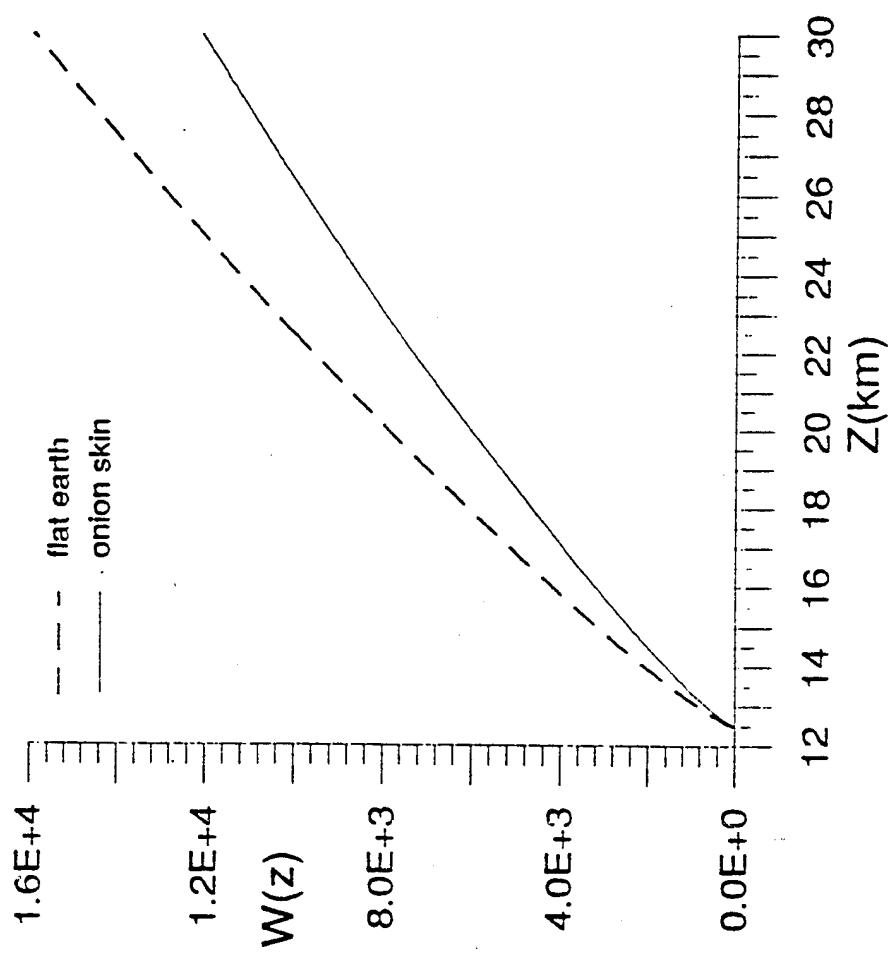
Then, for the Onion Skin Model, for propagation beginning at  $z_1$ :

$$W(z, \psi) = \left[ \sqrt{(R_e + z)^2 - (R_e + z_1)^2 \sin^2(\psi)} - (R_e + z_1) \cos(\psi) \right]^{\frac{5}{6}} \cdot \frac{0.56k^{\frac{7}{6}}(z + R_e)}{\sqrt{(z + R_e)^2 - (z_1 + R_e)^2 \sin^2(\psi)}}$$

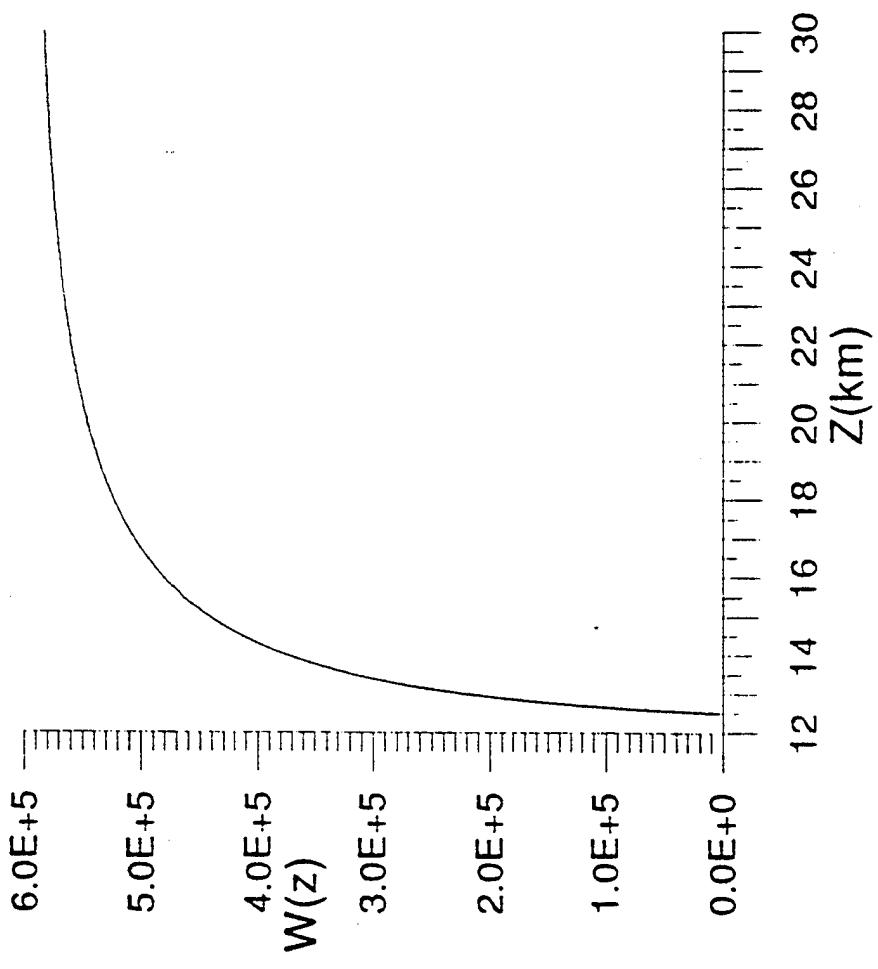
while for the Flat Earth model

$$W_F(z, \psi) = 0.56k^{\frac{7}{6}} \{ \sec(\psi) \}^{\frac{11}{6}} (z - z_1)^{\frac{5}{6}}$$

Plane wave altitude weighting function for zenith angle of  $60^\circ$



Plot of plane wave altitude weighting function for zenith angle of  $89^\circ$

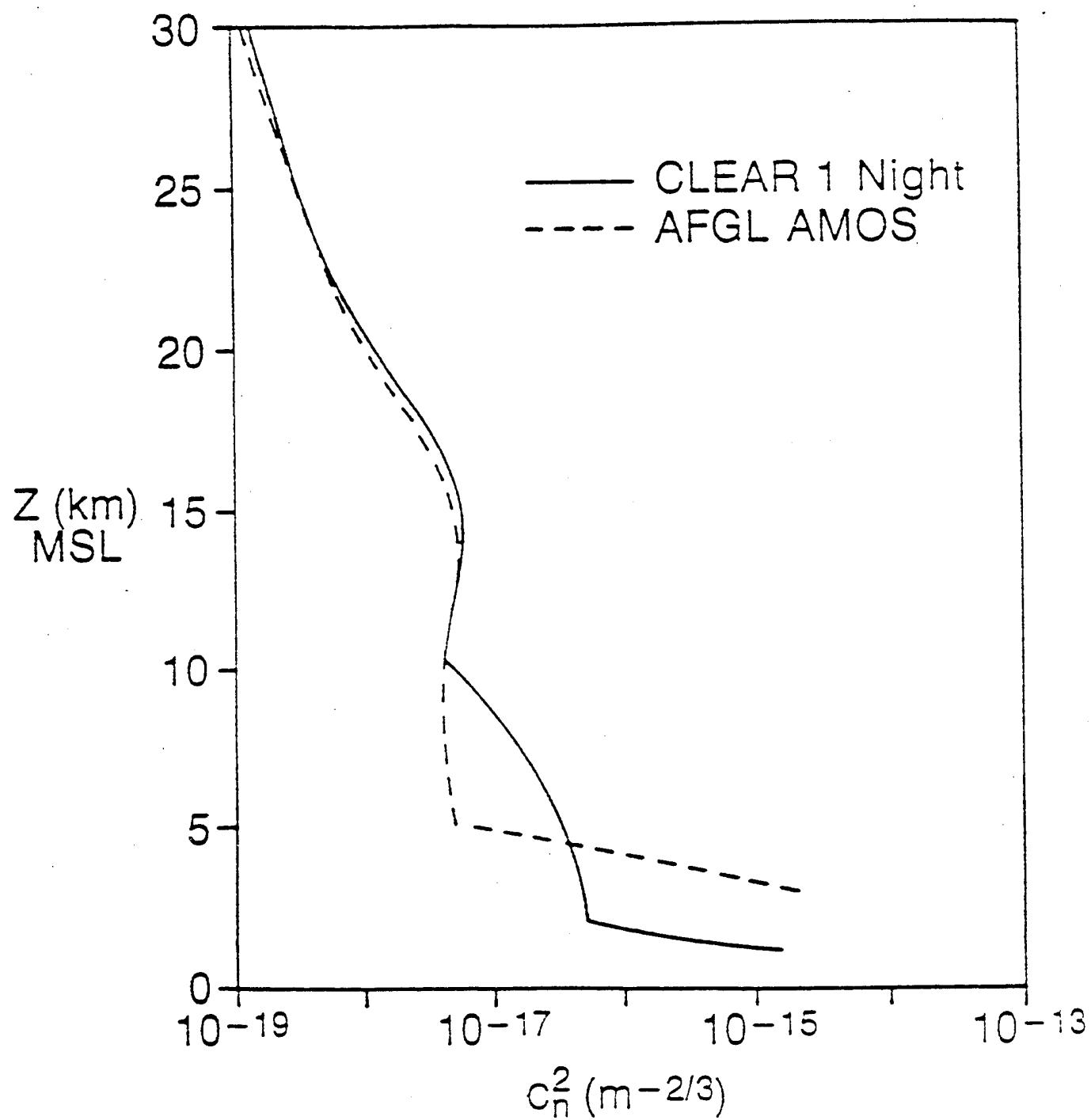


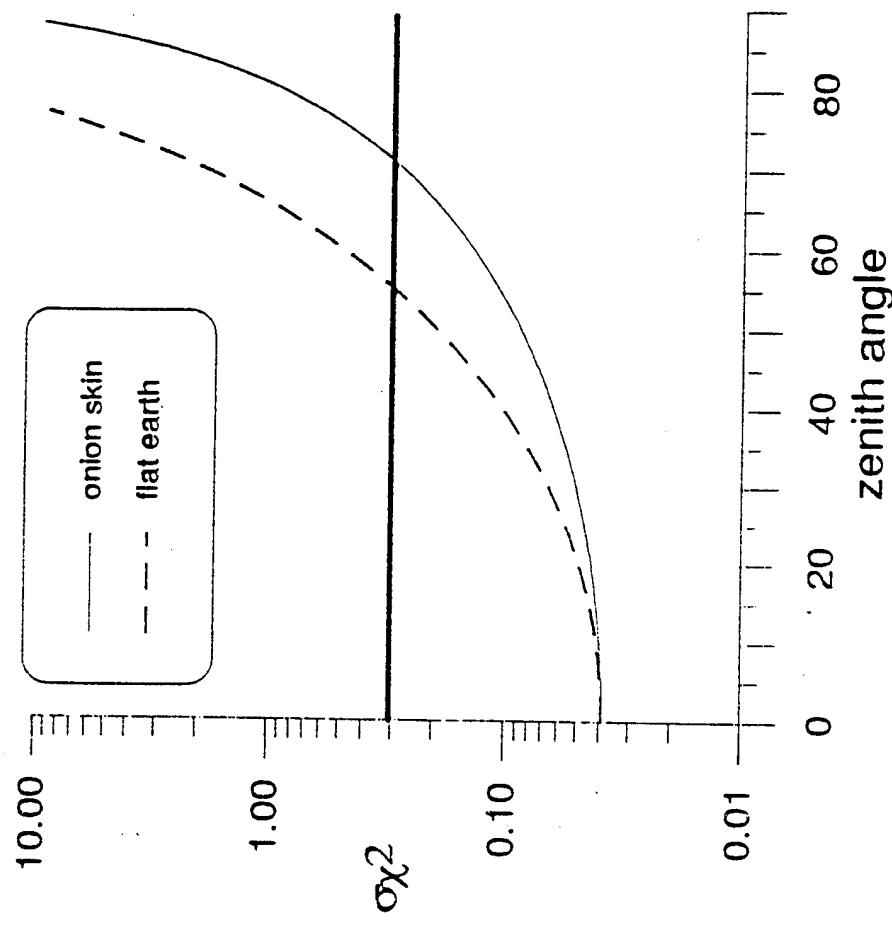
## Properties of $W(z, \psi)$

- Onion Skin and Flat Earth Model agree exactly at  $\psi = 0^\circ$
- Onion Skin and Flat Earth Model do not significantly differ for  $\psi < 30^\circ$
- For  $\psi = 90^\circ$ , Flat Earth Model is singular for all  $z$
- For  $\psi = 90^\circ$ , Onion Skin reduces to

$$W(z, 90) = 0.56k^{7/6} [(R_e + z)^2 - (R_e + z_1)^2]^{-1/2} (R_e + z)$$

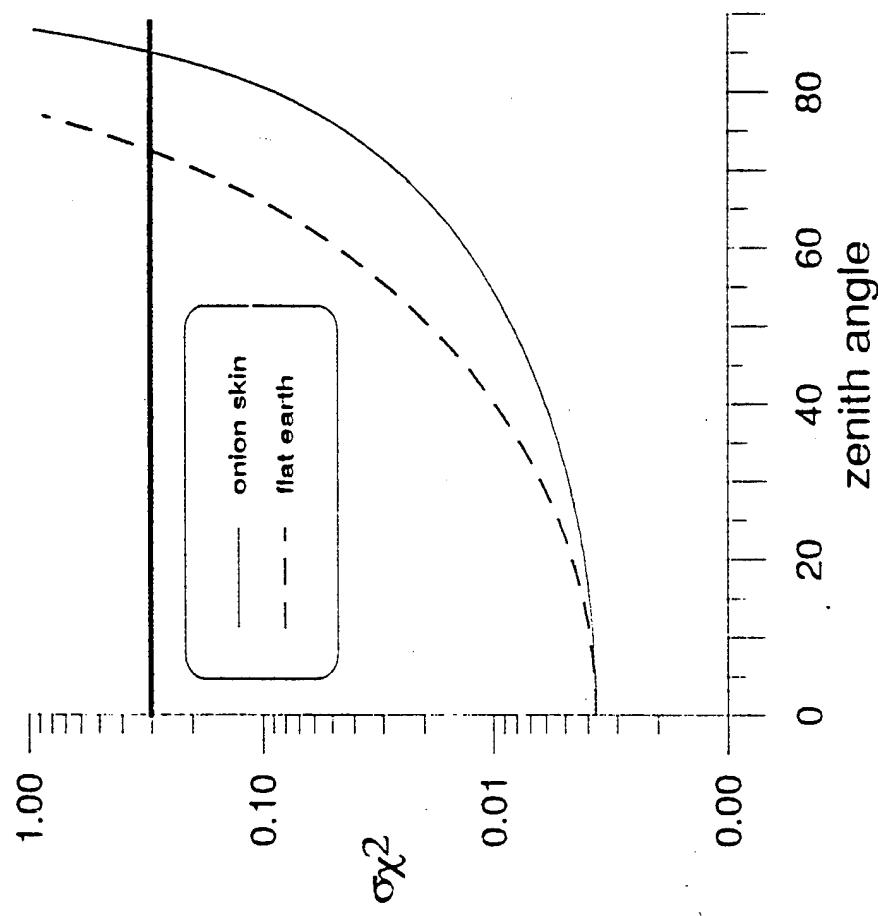
This has a weak singularity at the receiver,  $z_1$ . This is a mathematical singularity that is removed for any finite receiver aperture.





The turbulence profile used is that of CLEAR I.

The receiver is assumed to be at ground level (1.216 km MSL for CLEAR I). This calculation assumes a point receiver.



The turbulence profile used is that of CLEAR I.  
 The receiver is assumed to be at 12.5 km MSL.  
 This calculation assumes a point receiver.

## Finite Aperture Effects

For a receiver is a circular aperture of radius  $a$

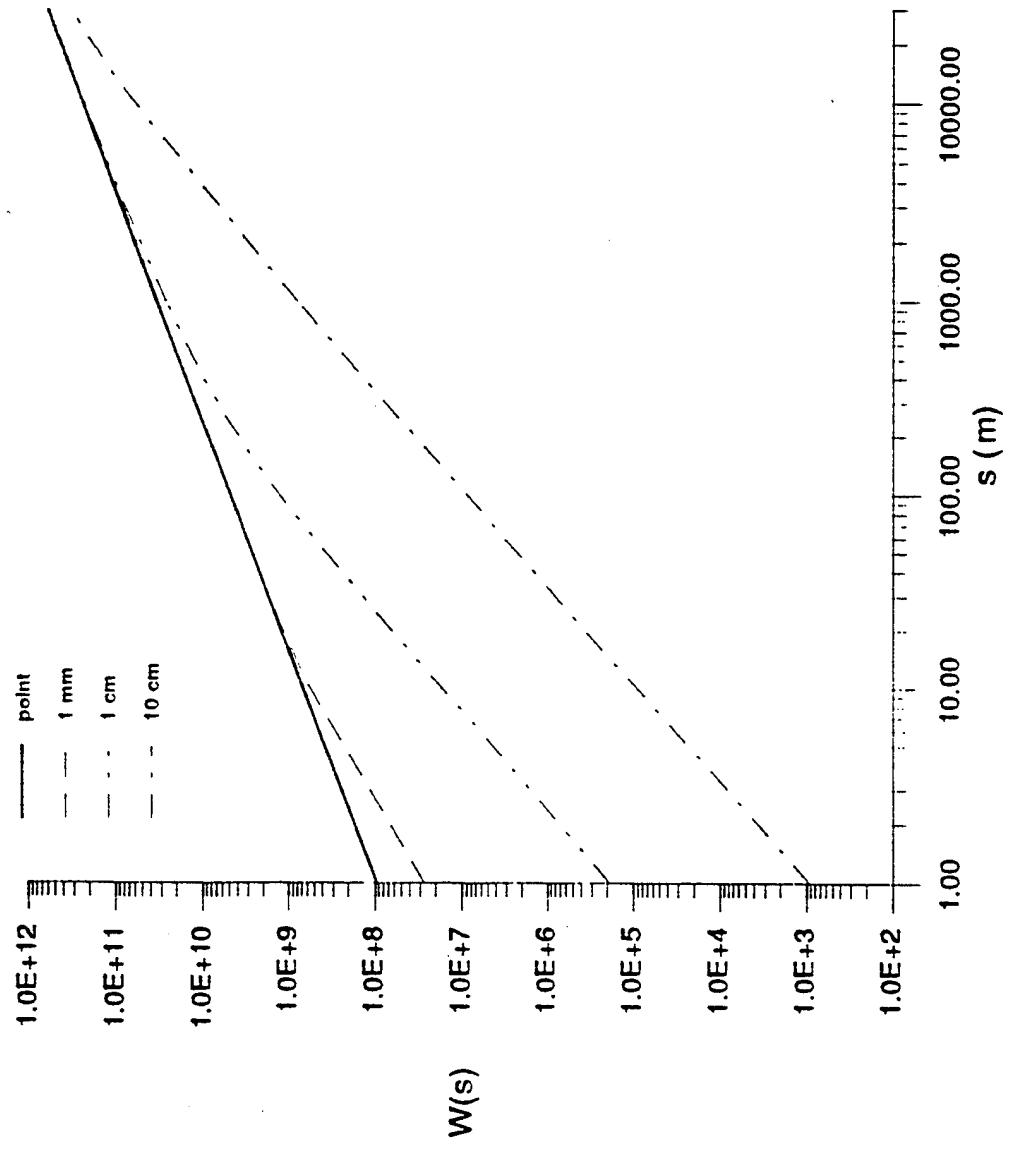
$$\sigma_{\chi}^2 = 4\pi^2 k^2 \int_0^L ds \int_0^\infty dK K \Phi_n(K, s) \sin^2 \left( \frac{K^2 s}{2k} \right) \left[ \frac{2J_1(Ka)}{Ka} \right]^2$$

Using Kolmogorov spectrum, we can define a path weighting function, as before:

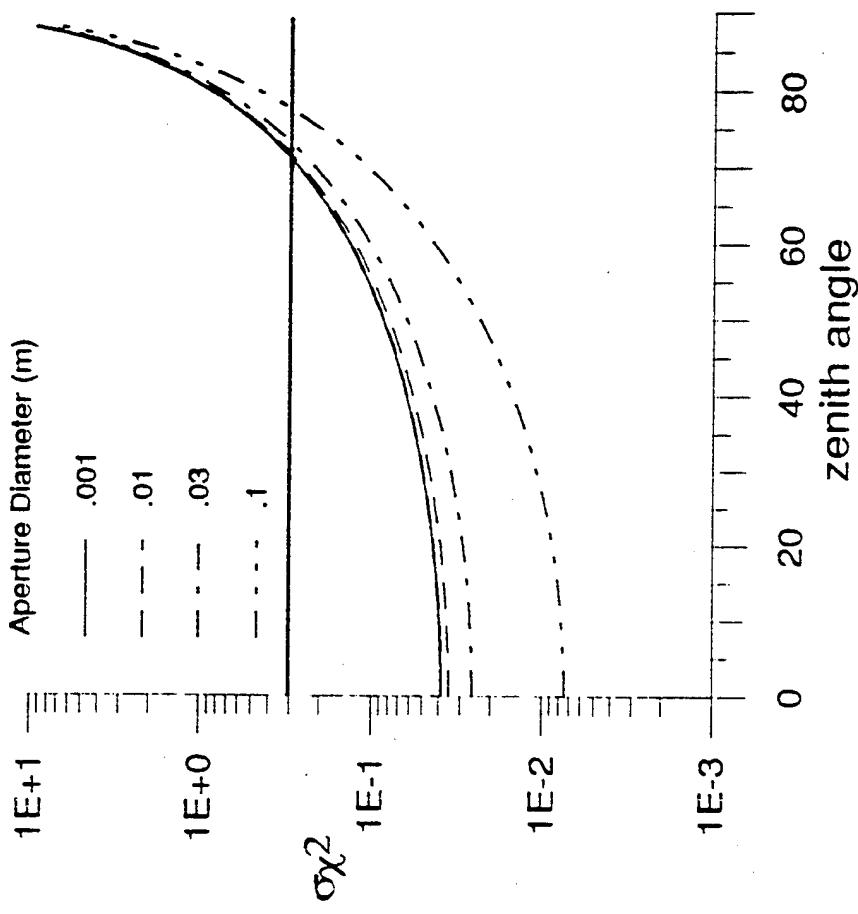
$$W(s, a) = 0.033\pi^2 2^{\frac{13}{6}} k^{\frac{1}{6}} a^{-2} s^{\frac{1}{6}} \int_0^\infty dK K^{\frac{-14}{3}} \sin^2(K^2) J_1(Ka \sqrt{\frac{2k}{s}})^2$$

and an Onion Skin altitude weighting function:

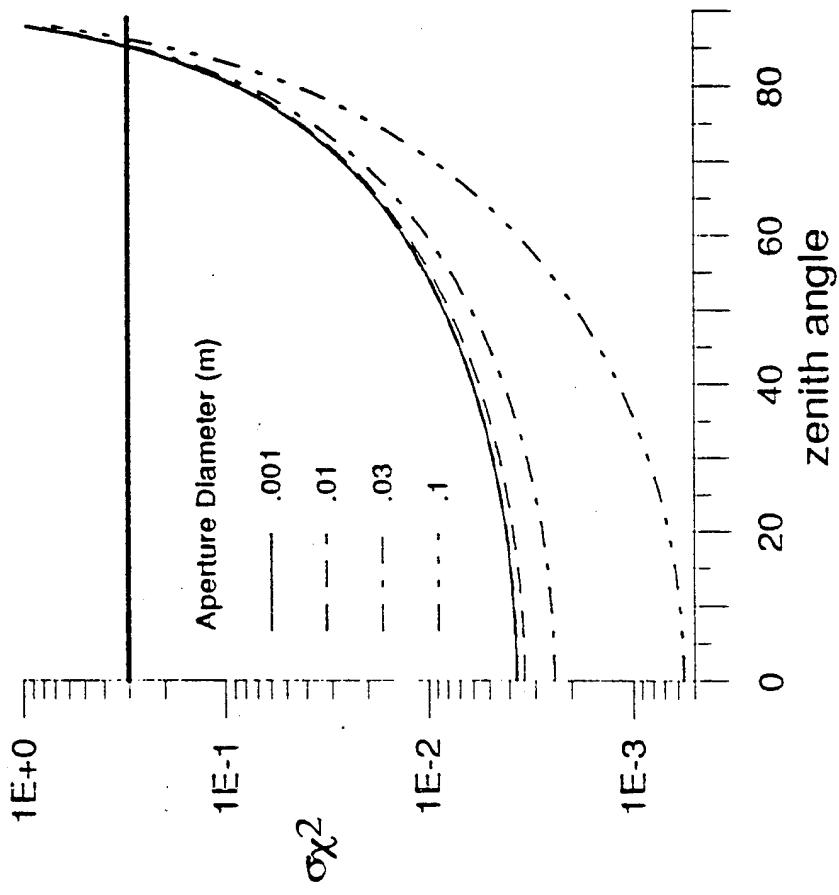
$$W(z, a, \psi) = 4\pi^2 k^2 f(z, \psi) \int_0^\infty dK K \Phi_0(K) \sin^2 \left( \frac{K^2 f(z, \psi)}{2k} \right) \left[ \frac{2J_1(Ka)}{Ka} \right]^2$$



Path weighting function for plane wave scintillation. The solid curve is the usual  $5/6$  power weighting function.



Plane wave log amplitude variance showing the effect of aperture averaging as a function of zenith angle. The calculation used the Clear I profile in an onion skin, with the receiver at ground level (1.216 km MSL).



Plane wave log amplitude variance showing the effect of aperture averaging as a function of zenith angle. The calculation used the Clear 1 profile in an onion skin model, with the receiver at an altitude of 12.5 km.

# Onion Skin Model Predictions for Airborne Measurements

- Rytov/onion skin model predicts
  1. that the weak fluctuation approximation applies to zenith angles  $< \approx 85^\circ$  and that larger angles are in the saturation region
- Rytov/Onion Skin model shows that there is a small difference between the 1 and 3 cm apertures at  $80^\circ$  (.08 vs .09) and explains the reduction of aperture averaging effect:
  1. Aperture averaging removes contribution from turbulence near the receiver.
  2. The reduction by a 1 cm aperture is due to the reduced contribution from the first km of the path. As the zenith angle increases, the atmospheric path increases and the ratio of the turbulence in the first kilometer to the rest of the path decreases.
  3. The amount of the reduction is a function of the distribution of the turbulence. A smooth distribution like CLEAR 1 produces different results than an actual profile that had a strong layer in the first kilometer of the path.

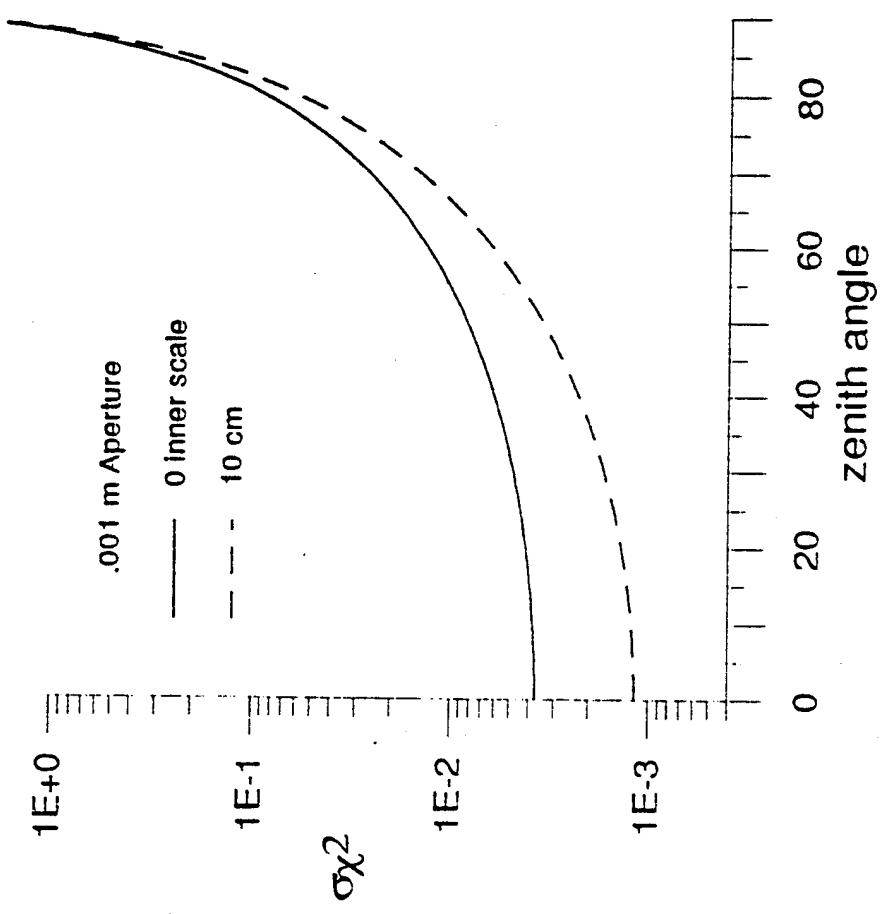
## Inner Scale Effects

- Non-zero inner scale effects can be included in the Rytov/Onion Skin Model by using the Tatarskii form of the spectrum

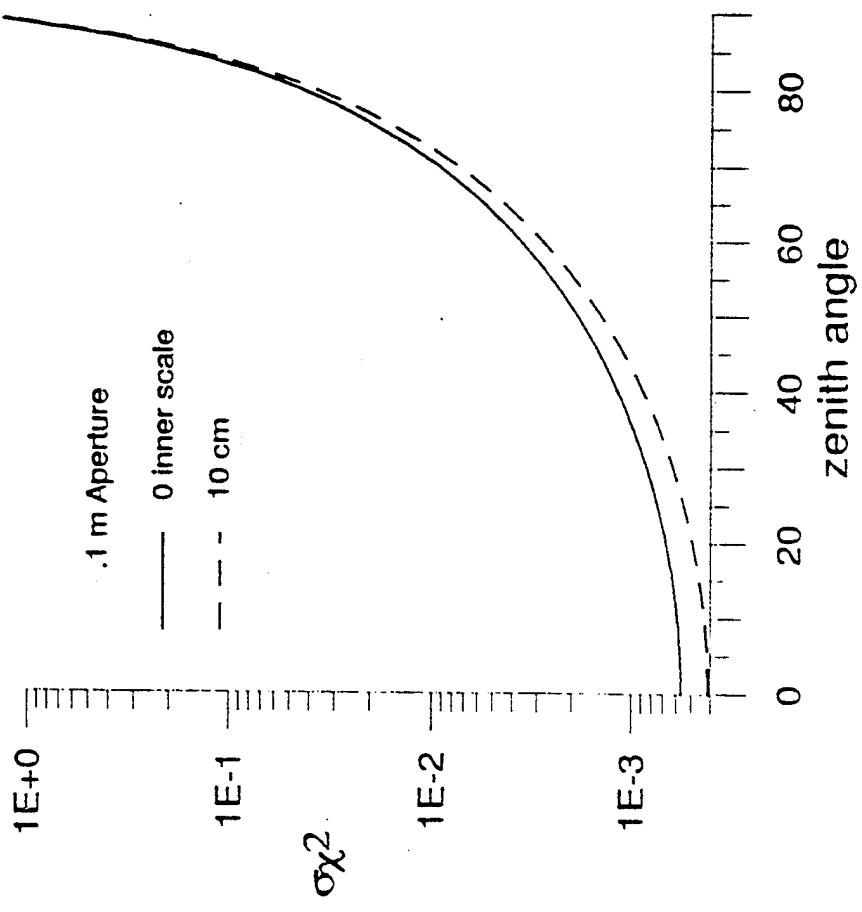
$$\Phi_n(K, s) = 0.033 C_n^2(s) K \frac{-11}{3} \frac{-K^2}{K_m^2}$$

where  $K_m = 5.92/l_0$  and  $l_0$  is the inner scale.

- Log amplitude variance will be calculated as before using this spectrum with  $l_0 = 10$  cm. This value is on the large side for propagation above 12.5 km, but should bound the problem.
- Inner scale is actually path dependent and increases with altitude. Only a constant value of 10 cm is used.



The effect of inner scale is shown for a 1 mm receiver. The calculation uses the Clear 1 profile and a receiver at 12.5 km altitude.



The effect of inner scale is shown for a 10 cm receiver. The calculation uses the Clear 1 profile and a receiver at 12.5 km altitude.

## Inner Scale: Results

In weak fluctuations and near horizontal propagation,

- inner scale is a small correction to log amplitude variance; it decreases in importance as the zenith angle increases (path length increases).
- When combined with aperture averaging, inner scale is further reduced in importance.

Why ? Just like the aperture averaging effect, small scales ( $< l_o$ ) contribute to log amplitude variance mainly from the part of the path in front of the receiver. This path forms less and less of the total turbulence as zenith angle increases. Of course, the relative magnitude of this contribution is determined by the distribution and strength of turbulence along the path.

BUT:

inner scale is very important to log amplitude variance in the strong or saturated scintillation domain.

## Comparison to Data

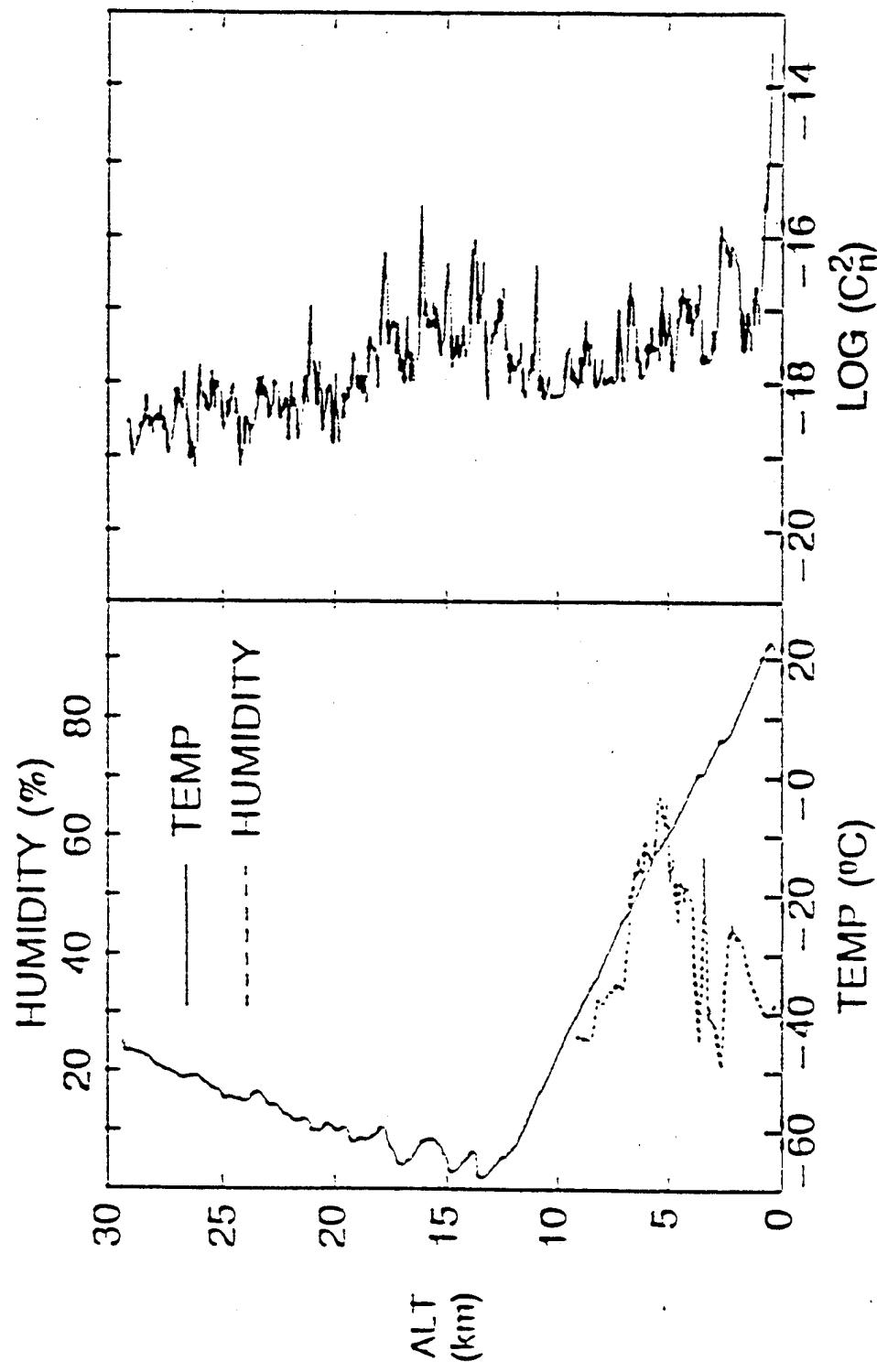
- The Rytov/onion skin model can be used to compare predictions with data for zenith angles as large as about  $85^\circ$ .
- Airborne measurements typically made from altitudes of 40,000-50,000 ft.
- Cn<sup>2</sup> profiles used were the Clear 1 model and actual PL/GP thermosonde profiles in order to include the effect of layering.
- Comparison of predictions to published astronomical data

## Profiles used

Name	location	trop hgt (km)	comments
CLEAR 1	WSMR	17	no layers; average
MT0575	Montana	9	winter
MT0582	Montana	9	winter
L4031	Penn State	13.5	low winds; strong layers
L4032	Penn State	11	jet stream
L3998	Cape Cod	12	jet stream
AZ8809	Azores	12.5	low trop and strat Cn2

L4031

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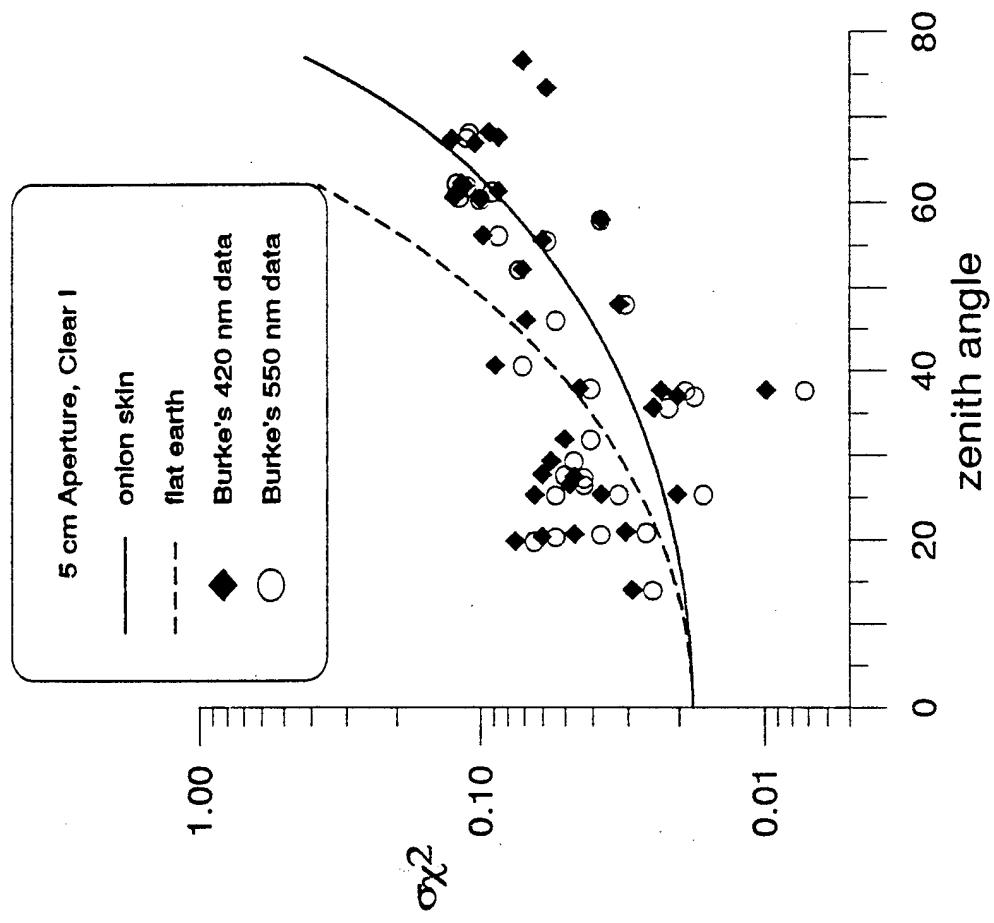


Predictions of  $\sigma\chi^2$  with Rytov/onion skin model

$d=0.3 \text{ m}$     $\lambda=0.5 \mu$     $z=50,200 \text{ ft}$     $\psi = 83.6^\circ$

Sirius (s105)

	$l_0=0$	$l_0=10 \text{ cm}$
Clear 1	0.036	0.025
MT0575	0.035	0.026
MT0582	0.042	0.031
L4031	0.139	0.098
L4032	0.089	0.069
AZ8809	0.039	0.031
L3998	0.049	0.039
data ave	0.066	0.049 +/-0.029
	+/-0.041	



Comparison of Burke's astronomical data (Burke,J.J., JOSA,**60**, 1262-1263,1960) with predictions using CLEAR 1 and an observer at ground (1.216 km MSL)

## Summary/Conclusions

- Onion skin formalism provides a model for horizontal structure of turbulence
- formalism reduces to "flat earth" model for small zenith angles and hence is an extension/refinement of the theory
- Predicts phenomena or behavior such as the reduction of inner scale and aperture averaging effects that are observed and not predictable from "flat earth" model
- Combined with Rytov theory, onion skin model yields expressions for near horizontal propagation that can be studied analytically
- formalism easily extended beyond plane wave scintillation to other optical effects such as spherical wave effects, image blurring and beam wander and broadening, etc

## Extensions

Fried's plane wave transverse coherence length:

$$r_0 = 2.1 \left[ 1.46k^2 \int_0^L C_n^2(s) ds \right]^{-3/5}$$

In the flat earth model,

$$r_0 = 2.1 \left[ 1.46k^2 \sec(\psi) \int_{z_1}^{z_2} C_n^2(z) dz \right]^{-3/5}$$

The coherence length in the onion skin model becomes

$$\begin{aligned} r_0 &= 2.1 \left[ 1.46k^2 \int_{z_1}^{z_2} C_n^2(z) f'(z, \psi) dz \right]^{-3/5} \\ &= 2.1 \left[ 1.46k^2 \int_{z_1}^{z_2} C_n^2(z) \frac{(R_e + z)}{\sqrt{(R_e + z)^2 - (R_e + z_1)^2 \sin^2(\psi)}} dz \right]^{-3/5} \end{aligned}$$

COMPARISON OF A MODEL DESCRIBING PROPAGATION THROUGH OPTICAL TURBULENCE (PROTURB) WITH FIELD DATA

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Physical Science Laboratory  
New Mexico State University  
Las Cruces, New Mexico 88003-0002

ABSTRACT

The PROTURB model, developed by the Battlefield Environment Directorate of Army Research Laboratory, calculates an estimate of optical turbulence strength and its effects on visible and infrared imaging and laser system performance. The PROTURB model was earlier compared to data obtained from the REBAL 92 field test held in Bushland, Texas, and data supplied by the Army Test and Evaluation Command Ft. Belvoir Meteorological Team<sup>1</sup>. Recent PROTURB updates included modifying the radiative flux portion of the energy balance model. Here we present a new comparison using data from three locations that differ greatly in meteorological conditions, including hot and moist conditions, hot and dry conditions, and moderate climatic conditions. There also exists a considerable difference in site characteristics such as ground conditions and vegetation. This latter data set was collected during the summer of 1993 at the following sites: Eglin AFB, Florida, Ft. Hunter-Liggett, California, and Ft. A.P. Hill, Virginia. We discuss the data collection and reduction effort, and show how this data compares with PROTURB predictions.

2. INTRODUCTION

The PROTURB model consists of five distinct modules; the PROTURB interface, surface boundary module, planetary boundary layer module, imaging statistics module and the laser propagation module. The PROTURB user-friendly interface controls the input of data, the calculation procedure and the display of the output data in both numerical and graphical form. The surface boundary layer module is based on a radiative-energy flux balance model<sup>3</sup>

that in turn drives a Monin-Obukhov similarity theory model<sup>2</sup> for unstable atmospheric conditions. This module is responsible for the optical turbulence profile that extends from 10 times the roughness length up to the Obukhov height. The surface boundary layer module takes into consideration the effects of moisture and gives approximations during stable atmospheric conditions and in and around the neutral events. The planetary boundary layer module is also based on Monin-Obukhov similarity theory and the Ekman spiral<sup>4</sup>. This module is responsible for the continuation of the optical turbulence profile from the Obukhov height to the top of the planetary boundary layer. The imaging statistics module is primarily based upon the work of D. L. Fried<sup>5</sup>. This module determines the image statistics that correspond to an image that has propagated over the designated path. The current laser propagation module is based on Rytov theory developed at ARL West<sup>6</sup>. This module is responsible for determining laser propagation statistics such as irradiance variance and beam size.

### 3. FIELD DATA COLLECTION

All field meteorological data were collected by the TECOM Ft Belvoir Meteorological Team. The same type of instruments were used at each location and proper calibration procedures were followed. Figure 1 locates the three locations. The optical

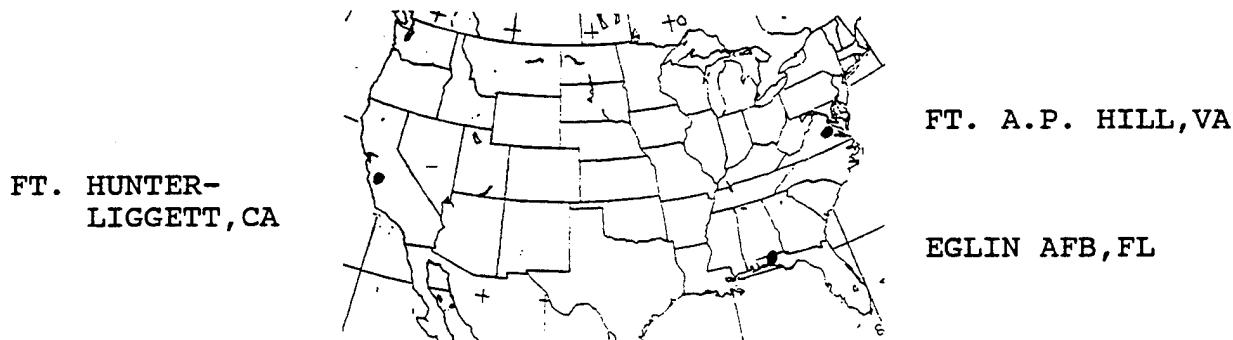


FIGURE 1 LOCATION OF DATA SITES

scintillometers used were the Lockheed model CN2. All data collection was automated and included temperature, relative humidity, pressure, rain rate and amount, visibility, soil temperature, long and short wave radiation, cloud amount, cloud height,  $C_n^2$ , and spectral atmospheric transmission. All data except clouds and transmission were collected in a single data set. An example is shown in table 1. Clouds and transmission were reported in separate files which are not shown here. It must be pointed out that in each case, the collection system was designed for the test support and not this comparison effort. The standard measurements were taken at a location very near the scintillometer receiver while the cloud data was taken from our base site which could be several kilometers away from the other measurements. Data from Ft.

Day	Time	Press	WDD	WSP	PKS	Temp	RH	Soil	Vsby	PSP	PSP	RNRT	SCINT	PIR	PIR
	hhmm	mb	dg	M/S	M/S	dg/c	%	dg/c	km	VER	CUT	mm/h	VOLT	VER	CUT
196	15 1012.8	143	0.35	0.60	23.2	94	14.9	10.54	0.00	0.00	0.00	0.016	391.5	442.4	
196	30 1012.6	20	0.04	0.40	23.1	95	14.8	9.15	0.00	0.00	0.00	0.013	390.8	441.7	
196	45 1012.6	52	0.09	0.40	23.1	95	14.6	10.86	0.00	0.00	0.00	0.005	391.1	441.5	
196	100 1012.4	104	0.21	0.60	23.1	95	14.6	11.51	0.00	0.00	0.00	0.017	390.2	440.3	
196	115 1012.3	60	0.31	0.90	23.0	95	14.5	9.81	0.00	0.00	0.00	0.012	390.8	440.4	

TABLE 1. FORMAT OF FIELD DATA

AP Hill and Eglin AFB were averaged for one minute while 10 minute data was collected at Ft. Hunter Liggett. Data was collected over the entire 24 hour period and examples of temperature, humidity, solar radiation and  $C_n^2$  are shown in figure 2 to illustrate the differences between the locations. Since much more data was collected than could possibly be used in this effort, a few representative days were chosen from each location. Complete details are available from the Ft. Belvoir team.

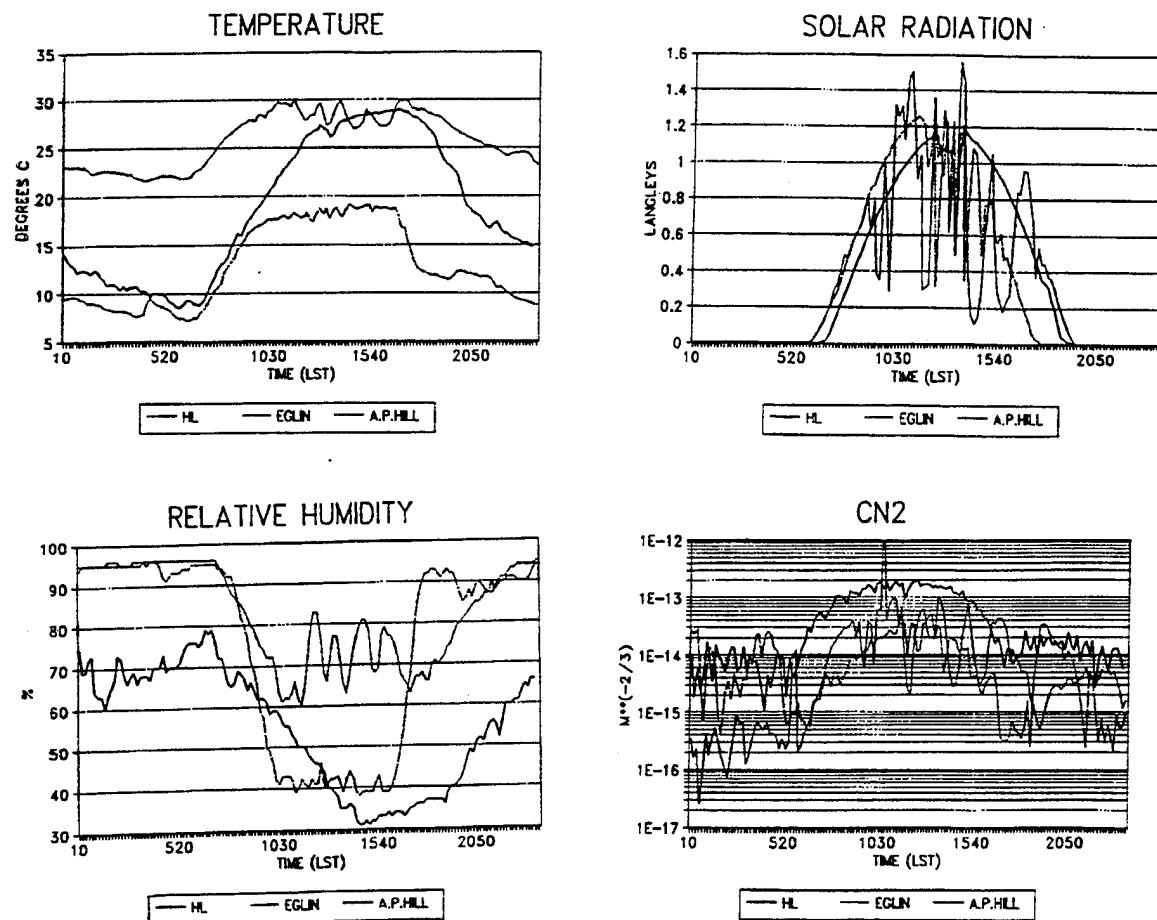


FIGURE 2 GRAPHICAL EXAMPLES OF SELECTED DATA EXAMPLES

#### 4. PROTURB METHODOLOGY

The field data was reviewed and 10 to 15 minute averages were determined. The geographical locations of the tests were determined to within 1/4 of a degree. The data point times were converted from local time to decimal GMT time. The original values for the relative humidity, wind speed, cloud properties and reference temperature were then converted to units acceptable to PROTURB. Table 2 and 3 are samples of the results of that effort. Table 2 is the time dependent inputs and Table 3 is an example of the PROTURB inputs with an identification of the various input.

Time GMT	Temperature degrees Kelvin	Wind Speed m/sec	Relative Humidity	Cloud Cover	Cloud Type	Cloud Density	Ceiling Height
2000	289.1500	6	0.94	99	0	4	1180
2025	288.9500	.7	0.94	99	0	4	900
2050	288.7500	1.1	0.94	99	0	4	700
2075	288.7500	.3	0.95	99	0	4	650
2100	288.7500	.3	0.95	99	0	4	200

TABLE 2 AN EXAMPLE OF METEOROLOGICAL DATA PREPARED FOR PROTURB

1993	9	8	35.8	-121.2	2100.0	20	1
600	285.00	310.25	973.0	2.0	0.416	2.0	0.05
0.26	50	3.0	10.0	1000.0	1.06	2	4
0.92	3	2	3	0	284.65	10.0	4.0
0.0	32.0	0	0				
LINE 1	LINE 2	LINE 3		LINE 4		LINE 5	
YEAR	CLOUD HGT	ALBEDO		GROUND EMISSIVITY		CUT OFF FREQ	
MONTH	REFERENCE TEMPERATURE	INTEGRATION SUB-INTERVAL	SOIL MOISTURE		FREQ CALC INTERVAL		
DAY	EST. MAX TEMPERATURE	RECEIVER HEIGHT	SOIL COMPOSITION		DEBUGGING FLAG		
LATITUDE	REFERENCE PRESSURE	SOURCE HEIGHT	VEGETATION FACTOR		PLANETARY EXTENTION FLAG		
LONGITUDE	WIND SPEED	PATH LENGTH	SNOW TYPE				
GMT	RELITIVE HUMIDITY	WAVE LENGTH	EST. MIN TEMPERATURE				
% CLOUD COVER	REFERENCE HEIGHT	CLOUD TYPE	FOCAL LENGTH				
GROUND COVER	ROUGHNESS ELEMENT	CLOUD DENSITY	ENTRANCE PUPIL DIA.				

TABLE 3 AN EXAMPLE OF A PROTURB INPUT DATA SET

The unstable atmosphere diurnal output from the PROTURB model was then compared to the corresponding measured values for Cn2 and the incoming solar radiation. Error analysis was performed

on the unstable atmospheric condition portion of the numerical results.

Incomplete knowledge of the test site forced the assumption of some of the values for the air pressure, the soil characteristics, and the vegetation characteristics. These values were estimated through the use of site photographs, topographic maps and data from surrounding sites. The most critical of these inputs is the estimation of soil wetness which was estimated through the use of rainfall data and on-site observations. The beam path was considered to be a constant height of 2.0 meters above the ground. The remaining parameters are presented above in the sample input cards.

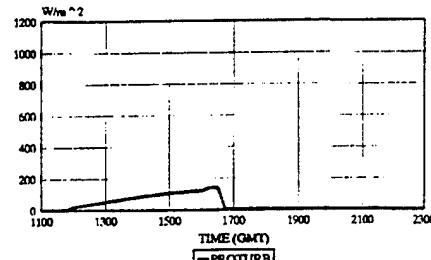
## 5. RESULTS

The results of the comparisons are presented in Figures 3 through 5 which show both the  $C_n^2$  and the incident shortwave radiation. Figure 3 shows comparisons from Ft. AP Hill. Agreement in solar radiation is very good. The  $C_n^2$  does show some large differences but are still considered good when one considers the terrain of the path. The comparisons do show a vast improvement over the predecessor model "IMTURB" as discussed by Smith and Corbin<sup>1</sup>. Figure 4 shows Ft. Hunter-Liggett data which also looks quite good. The deviation shown on 6 September is probably due to differing cloud conditions between the base site and the observation site 3 kilometers away. Figure 5 shows Eglin AFB data. Here the cloud observation was 6 km from the data site. Again the agreement is considered very encouraging. If perfectly representative data were available, better agreement would be expected.

The daylight portion of the error analysis is presented in Tables 4 and 5. These results include only times when the atmosphere was unstable. The percent  $C_n^2$  variation was determined by the relation %Variation =  $100.0 * ((\text{Measured}-\text{PROTURB})/\text{Measured})$ . The mean, standard variation, standard error and skewness of the percent variations were then determined. The radiation difference is presented in units of watts/meter<sup>2</sup> and is a straight difference between the measured and calculated values.

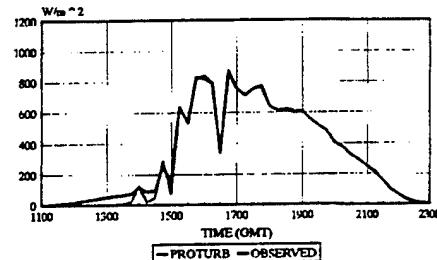
The values for percent variation of  $C_n^2$  at Ft. A. P. Hill were quite large and negative. The negative values are an indication that the PROTURB model predicted larger  $C_n^2$  values than were measured. The negative values for the skewness also indicates the presence of a systematic error. It is believed that the main source of error is in the estimation of a 2.0 meter height for the scintillometer positions. The actual site possessed several shallow canyons along the propagation path. This would mean that the actual average path height was greater than

INCIDENT SHORTWAVE RADIATION, FT. A.P. HILL, Va.  
PROTURB vs. OBSERVED - (OBSERVED IS MISSING)



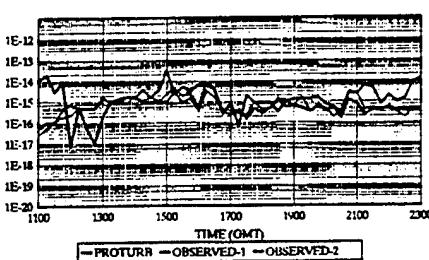
Date: 25 September 1993

INCIDENT SHORTWAVE RADIATION, FT. A.P. HILL, Va.  
PROTURB vs. OBSERVED



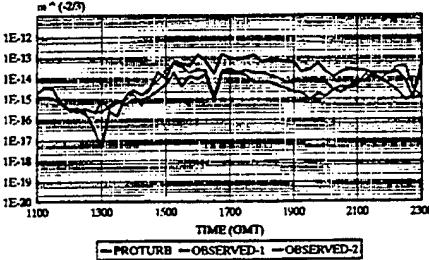
Date: 26 September 1993

Cu<sup>2</sup> COMPARISON, FT. A.P. HILL, Va.  
PROTURB vs. OBSERVED



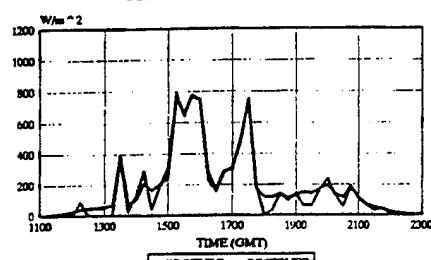
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Cu<sup>2</sup> COMPARISON, FT. A.P. HILL, Va.  
PROTURB vs. OBSERVED



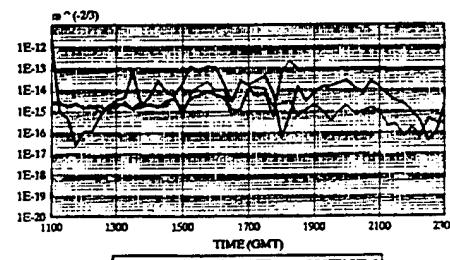
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INCIDENT SHORTWAVE RADIATION, FT. A.P. HILL, Va.  
PROTURB vs. OBSERVED



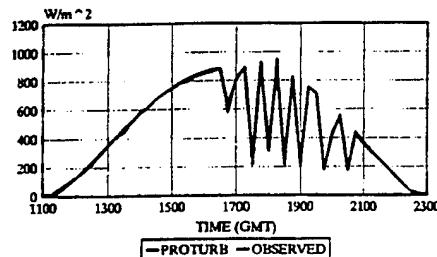
Date: 27 September 1993

Cu<sup>2</sup> COMPARISON, FT. A.P. HILL, Va.  
PROTURB vs. OBSERVED



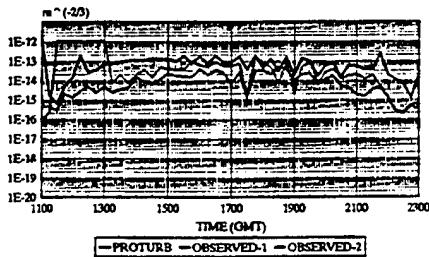
Date: 27 September 1993

INCIDENT SHORTWAVE RADIATION, FT. A.P. HILL, Va.  
PROTURB vs. OBSERVED



Date: 29 September 1993

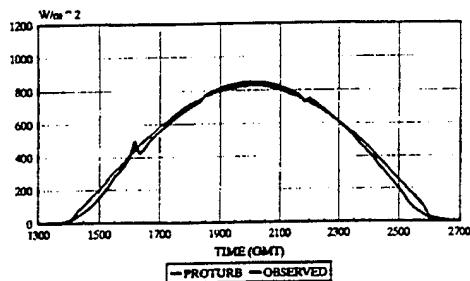
Cu<sup>2</sup> COMPARISON, FT. A.P. HILL, Va.  
PROTURB vs. OBSERVED



Date: 29 September 1993

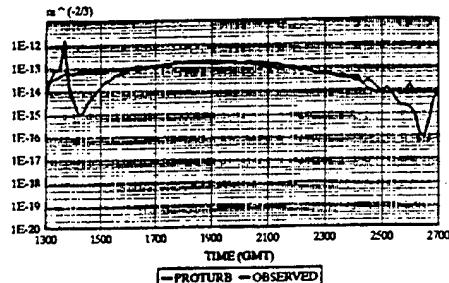
FIGURE 3. COMPARISONS FROM FT A.P. HILL, VA

INCIDENT SHORTWAVE RADIATION FT HUNTER-LIGGETT, CA.  
PROTURB vs. OBSERVED



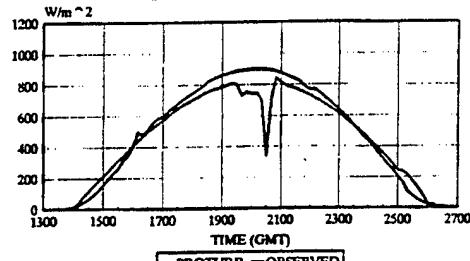
Date: 4 September 1993

Ca<sup>2</sup> COMPARISON FT. HUNTER-LIGGETT, CA.  
PROTURB vs. OBSERVED



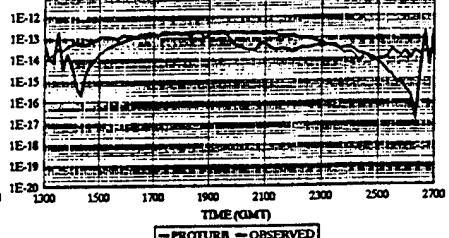
Date: 4 September 1993

INCIDENT SHORTWAVE RADIATION FT. HUNTER-LIGGETT, CA. Ca<sup>2</sup> COMPARISON, FT. HUNTER-LIGGETT, CA.  
PROTURB vs. OBSERVED



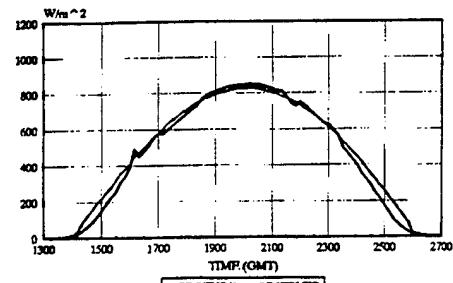
Date: 6 September 1993

Ca<sup>2</sup> COMPARISON, FT. HUNTER-LIGGETT, CA.  
PROTURB vs. OBSERVED



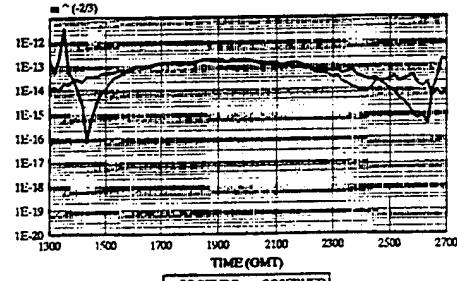
Date: 6 September 1993

INCIDENT SHORTWAVE RADIATION, FT. HUNTER-LIGGETT, CA.  
PROTURB vs. OBSERVED



Date: 8 September 1993

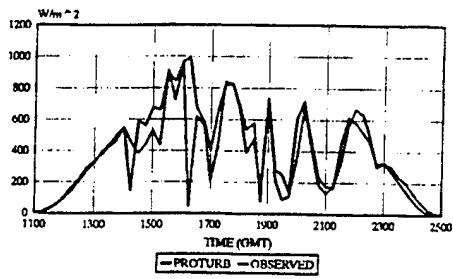
Ca<sup>2</sup> COMPARISON, FT. HUNTER-LIGGETT, CA.  
PROTURB vs. OBSERVED



Date: 8 September 1993

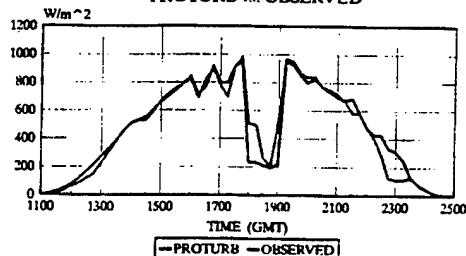
FIGURE 4. COMPARISONS FROM FT HUNTER-LIGGETT, CA

INCIDENT SHORTWAVE RADIATION, EGLIN AFB, FL.  
PROTURB vs. OBSERVED



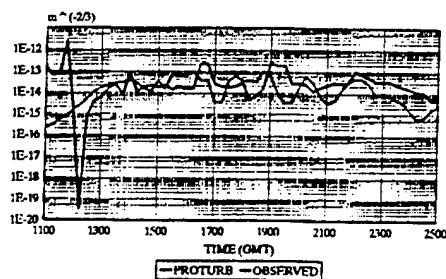
Date: 15 July 1993

INCIDENT SHORTWAVE RADIATION EGLIN AFB, FL.  
PROTURB vs. OBSERVED



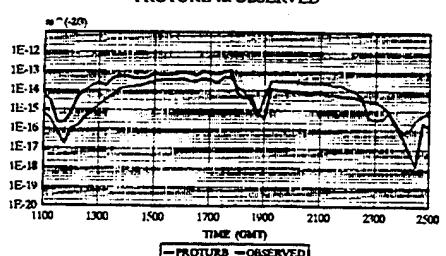
Date: 22 July 1993

C<sub>n</sub><sup>2</sup> COMPARISON EGLIN AFB, FL.  
PROTURB vs. OBSERVED



Date: 15 July 1993

C<sub>n</sub><sup>2</sup> COMPARISON EGLIN AFB, FL.  
PROTURB vs. OBSERVED



Date: 22 July 1993

FIGURE 5. COMPARISONS FROM EGLIN AFB, FL

Test Name	Mean $\pm C_n^2$ Variation	Standard Deviation	Standard Error	Skewness
A.P. Hill day 268	-254.929	484.5339	77.58751	-2.53145
A.P. Hill day 269	-310.992	396.5045	57.23050	-1.16931
A.P. Hill day 270	-869.412	1247.6720	180.08600	-1.82635
A.P. Hill day 272	-1285.680	1506.9560	217.51030	-2.19559
Pt. H-L day 247	6.5033	49.03060	5.587556	0.01920
Pt. H-L day 249	25.3578	51.54052	6.599088	-1.26270
Pt. H-L day 251	-20.3807	90.60885	11.06963	-2.32109
Eglin AFB day 196	-352.167	908.3837	128.3668	-4.95832
Eglin AFB day 203	-136.794	285.4617	43.03498	-2.44425

TABLE 4. C<sub>n</sub><sup>2</sup> Variation statistics. Data points that indicate stable or neutral conditions have been excluded from the statistical analysis. Also, experimental data that indicate equipment malfunction have been excluded.

Test Name	Mean Difference	Standard Deviation	Standard Error	Skewness
A.P. Hill day 268	NA	NA	NA	NA
A.P. Hill day 269	-11.2668	24.33080	3.511848	-1.32431
A.P. Hill day 270	-16.7757	41.56963	6.000059	-0.34138
A.P. Hill day 272	-5.7251	18.67955	2.696161	0.17929
Pt. H-L day 247	6.5033	49.03060	5.587556	0.09030
Pt. H-L day 249	-24.2058	83.466530	9.053083	-3.27868
Pt. H-L day 251	16.5451	33.65205	3.587320	0.55062
Eglin AFB day 196	-33.6366	157.24060	21.01214	-3.60090
Eglin AFB day 203	-1.83572	85.89066	11.47762	1.37096

TABLE 5. Short wave radiation difference statistics.

2.0 meters. An increase in the assumed path height would reduce the  $C_n^2$  values generated by PROTURB thus reducing the error. The occurrence of fog and rain along the path should also be considered a source of error since PROTURB does not include the actions of such atmospheric additives. In general, the PROTURB values tend to possess the same trends as the measured values and though the error is quite high the results are comparable with that of models with similar input simplicity.

The values for percent variation of  $C_n^2$  at Ft. Hunter-Liggett were very reasonable. There appears to a sea breeze effect present in the measured data in both the morning and afternoon. The PROTURB model assumes that the atmospheric condition is generated by the surface-air interface and not influenced by outside forces such as weather fronts and nearby surface inhomogeneities such as a land-sea interface. Thus the prevailing deviations were seen in the morning and early evening were less pronounced possibly due to the effect of the nearby ocean. The surface at Ft. Hunter-Liggett was relatively flat leading to better overall results.

The values for percent variation of  $C_n^2$  at Eglin AFB, were moderately successful. The PROTURB model was more sensitive to wind speed and cloud coverage than the measured data. In general, PROTURB would have predicted larger values for results had it not been for this sensitivity. The over prediction of  $C_n^2$  can be attributed to PROTURB'S lack of sensitivity in relation to soil type and soil moisture effects. An upgraded soil model is currently under development and should be installed by the time of public release.

The shortwave radiation comparison at all sites were very good. The primary deviation is in the shape of the clear-sky curve directly after sun rise and before sunset. This greater measured radiation at these points can be assumed to be related to the value of the diffuse sky radiance at low solar elevation angles. It appears that the PROTURB cloud reduction factors represent reasonable approximations to the effects of clouds.

A more complete analysis is being prepared for the use of the Army Research Laboratory by Cranston and Cruncleton.

#### CONCLUSIONS

Given that some necessary approximations were made in transforming from a nonuniform terrain to a uniform terrain with fixed site parameters, the PROTURB model did a reasonable job in the determination of  $C_n^2$ . It was noticed that the significant decreases and increases in  $C_n^2$ , due to clouds and wind effects,

are parallel in both PROTURB and measured values, but that the PROTURB model appears to be overly sensitive to these factors. The primary factors responsible for this sensitivity are the Angus-Leppan wetness and cloud parameters, and the thermal diffusivity of the soil. These factors play important roles in the energy partition within the energy balance model and should be scrutinized further. The comparisons presented here considered only the unstable condition. Noting the collected turbulence data

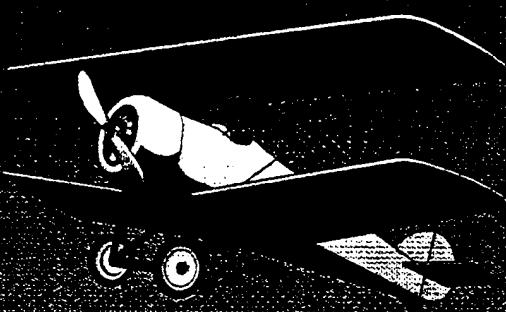
shown on figure 2, it is recommended that an effort be made to extend the model into night or stable conditions.

#### References

1. R. W. Smith and T. Corbin, "Field measurement and comparison of optical turbulence.", SPIE Vol. 1687
2. W. B. Miller and J. C. Ricklin, "A Module for Imaging Through Optical Turbulence - IMTURB", U. S. Army Atmospheric Sciences Laboratory Tech Report - 0221-27, November 1990.
3. H. Rachele and A. Tunick, "Energy Balance Model for Imagery and Electromagnetic Propagation", U. S. Army Atmospheric Sciences Laboratory Tech Report - 0311, May 1992.
4. H. Rachele, "Ekman Spiral", unpublished notes, April 20 1992.
5. D. L. Fried, "Theoretical Study of Non-Standard Imaging Concepts", Defense Technology Information Center Tech Report - RADC-TR-76-51, March 1976.
6. W. B. Miller, J. C. Ricklin and L. C. Andrews, "Log-amplitude variance and wave structure function: a new perspective for Gaussian beams", Journal Optical Society of America, Vol.10, No.4, April 1993.

# TURBULENCE IS A FEATURE OF MOST CLOUDS

Surf  
intense than  
others



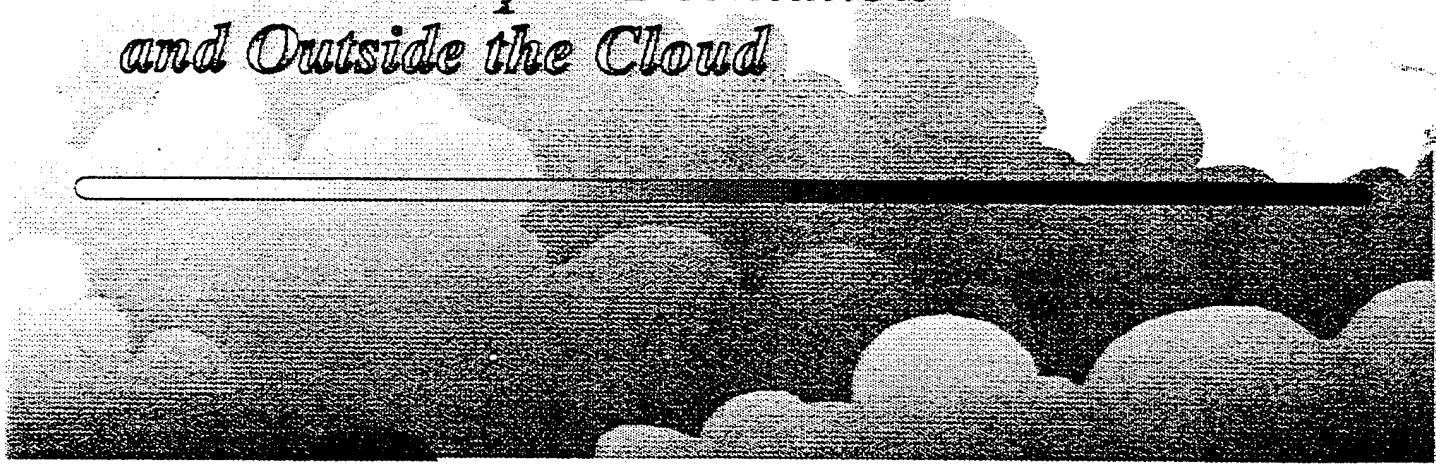
J.W. TELFORD

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# THE ROLE OF TURBULENCE

*in Cloud Droplet Formation  
and Outside the Cloud*

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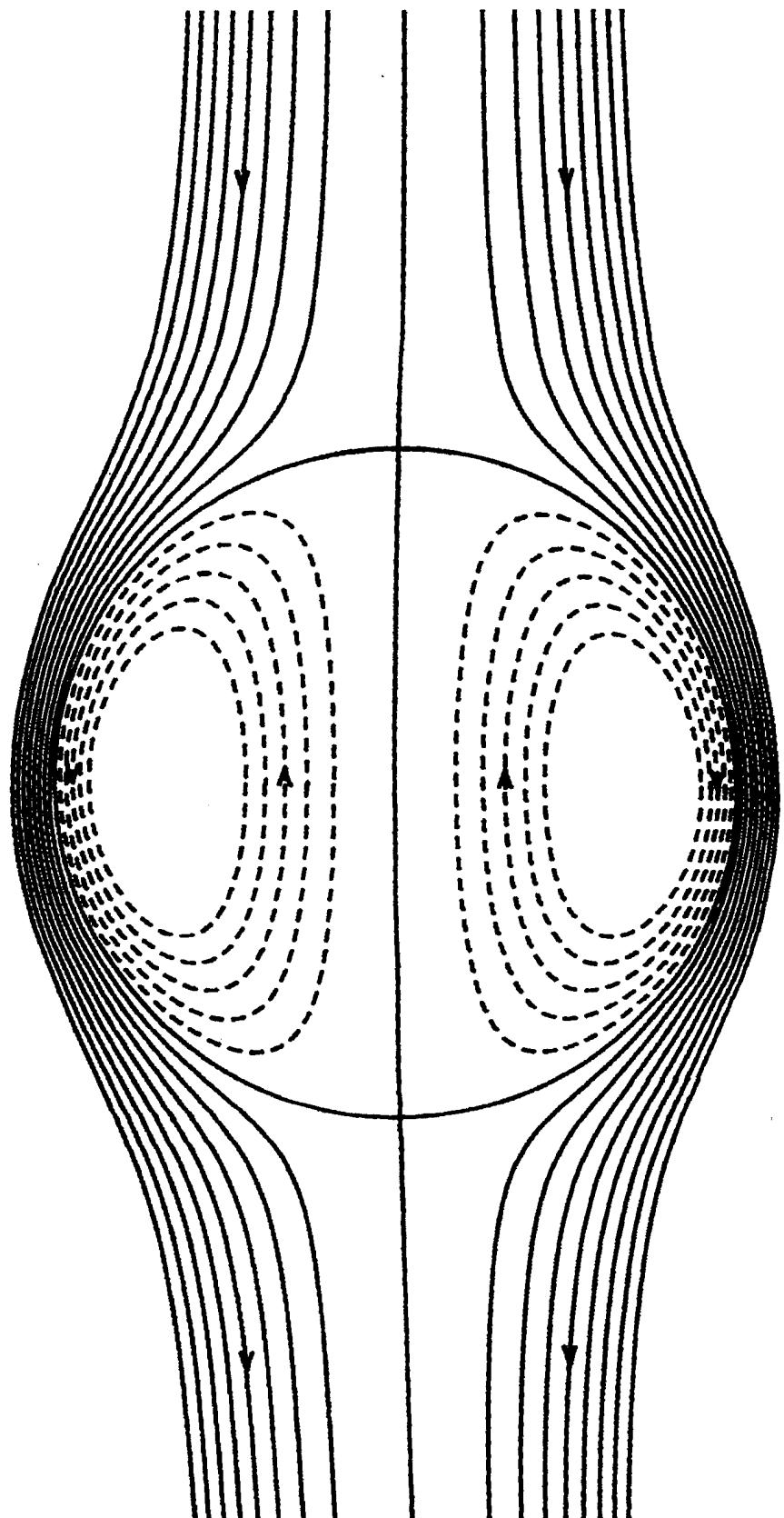


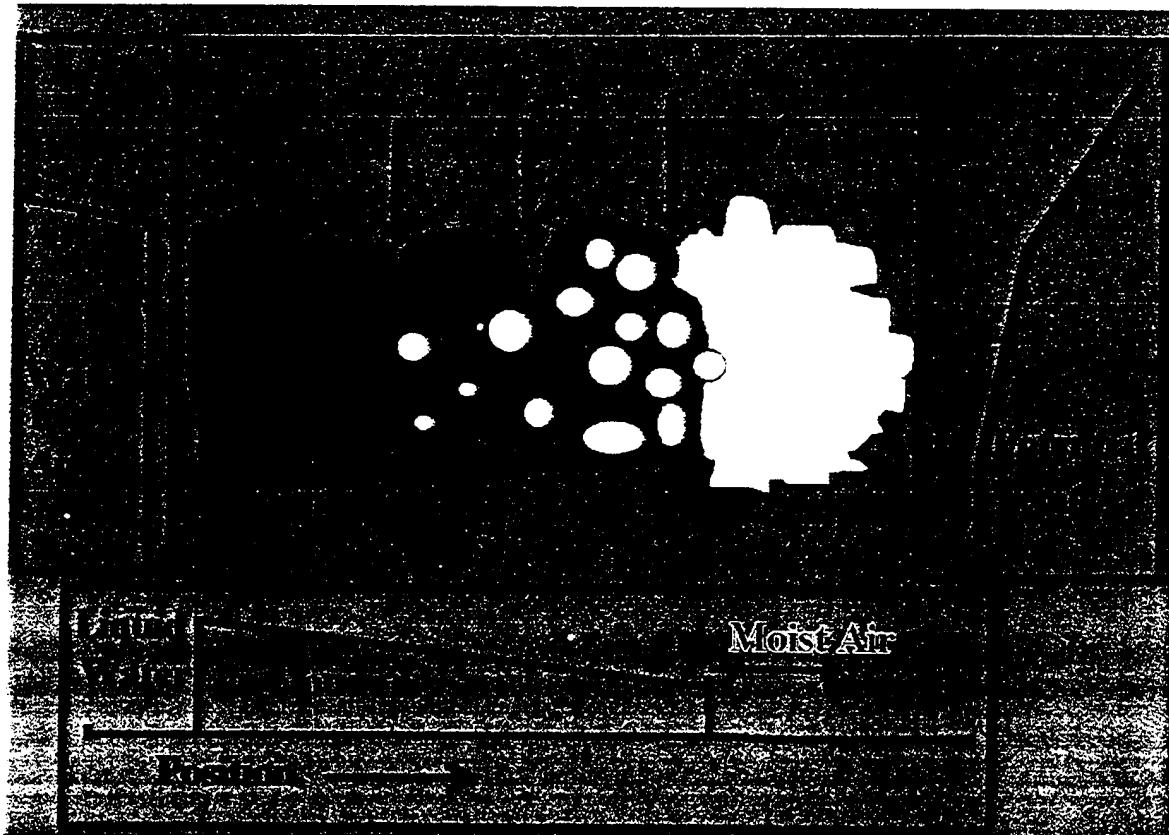
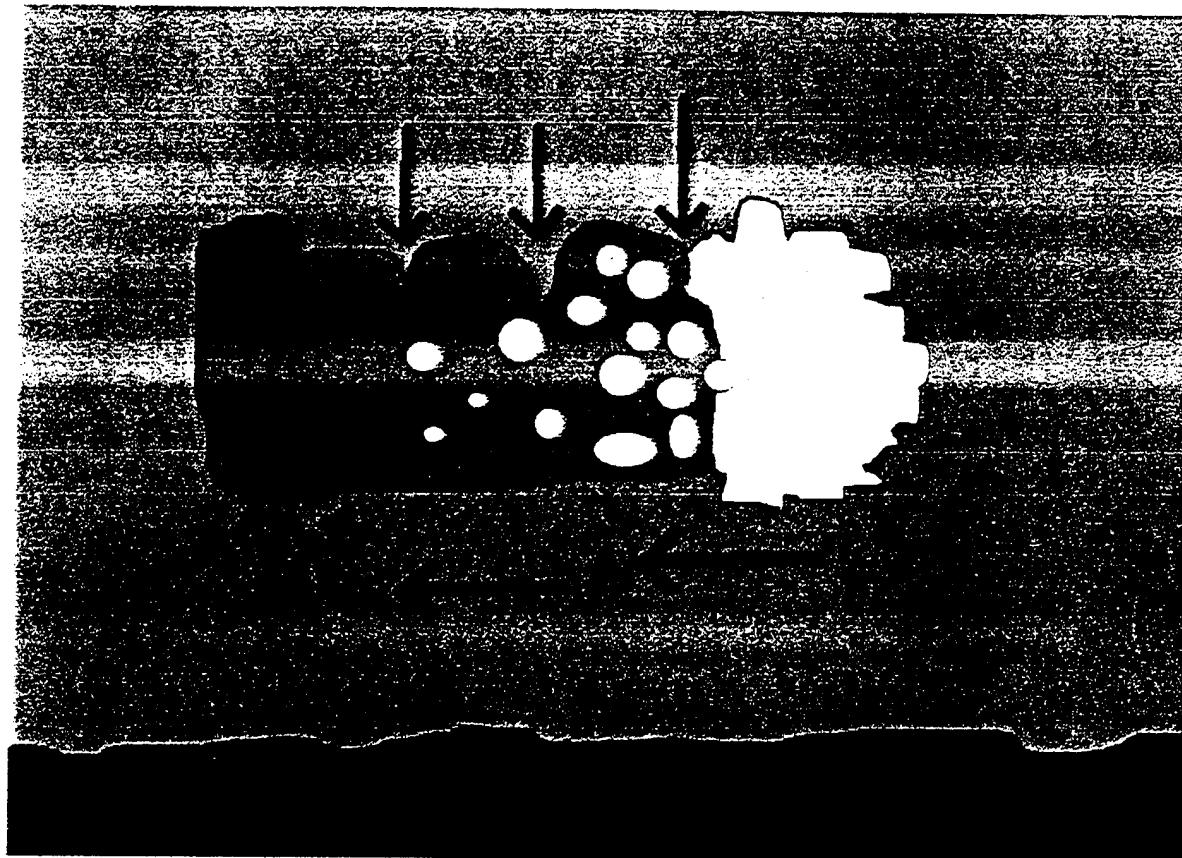
The possible exception to the general turbulence of clouds are the wave clouds formed in the rising wave flow near mountains. The cloud forms in the upflow and evaporates in the downflow after the crest. Such clouds lack the buoyant updrafts and downdrafts which generate turbulence.

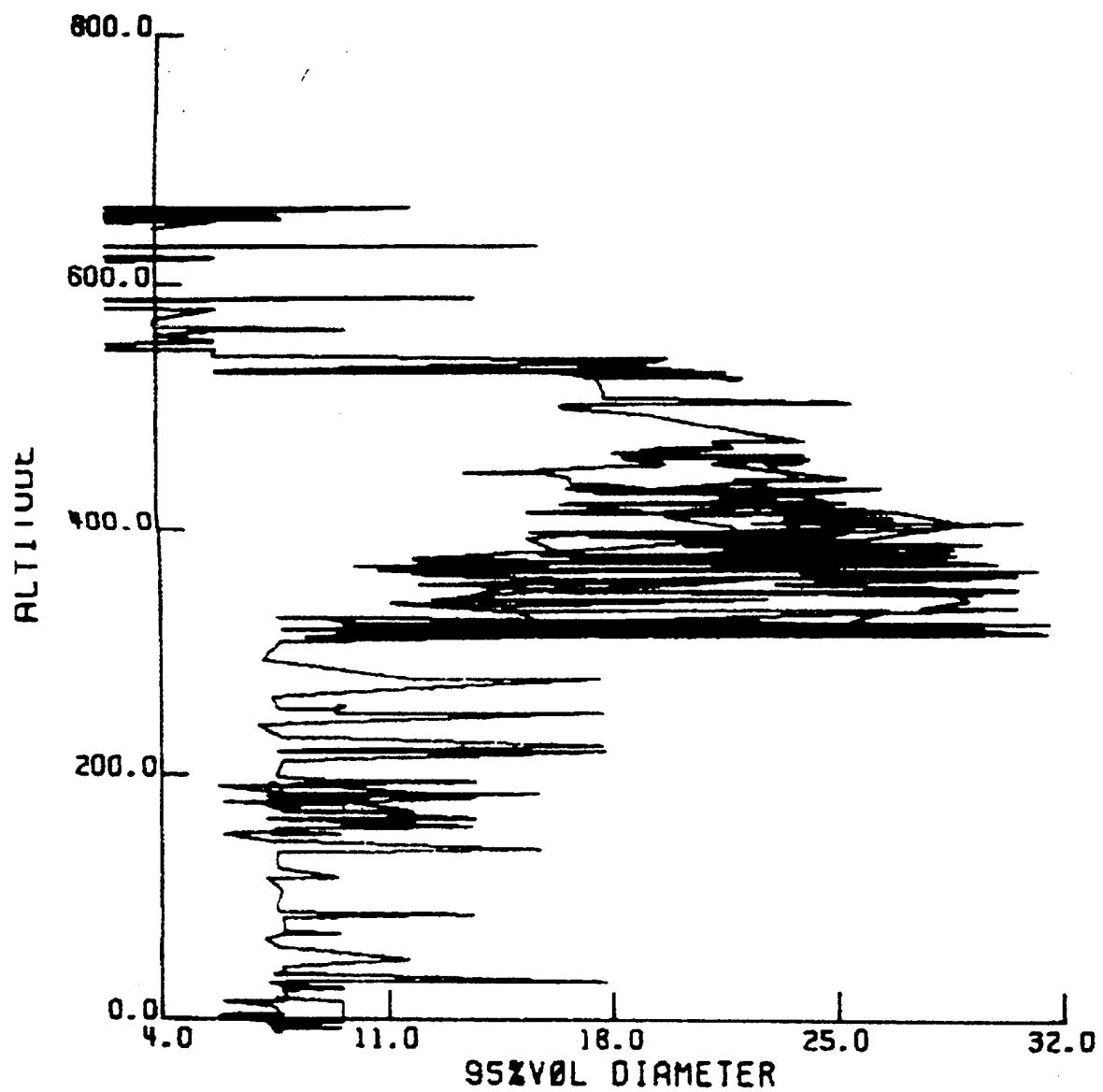
Wave clouds are common in certain areas where cold air moves over warm land or water. They form in the upflow and evaporate in the downflow behind them which builds up very severe turbulence from contact with the ground. When cloudy, these clouds probably have the most severe turbulence of any clouds.

Stratus clouds are diluted by descending turbules which bring water vapor and ambient cloud tops into the clouds. These clouds in storms have more than 10% water droplets. This is the cause of

These turbules modify the cloud microphysical particles to such an extent that this is the primary controlling factor.

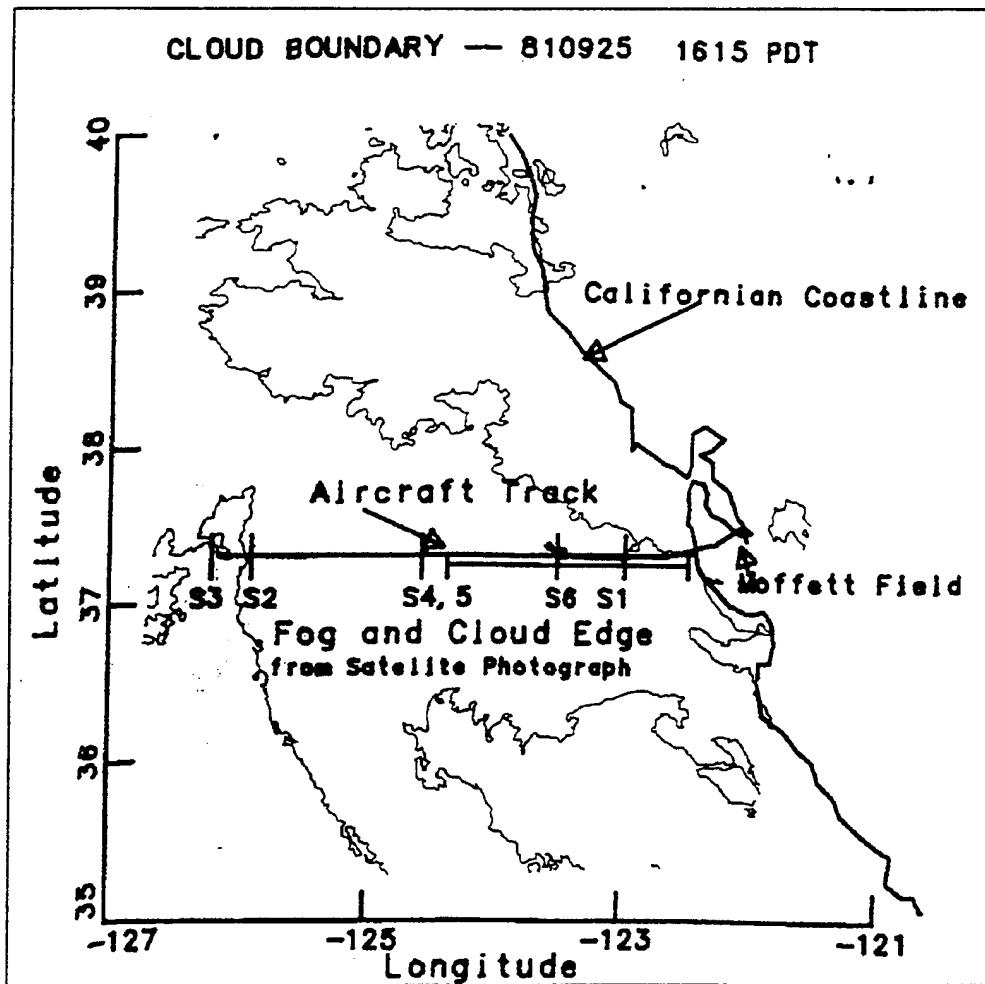




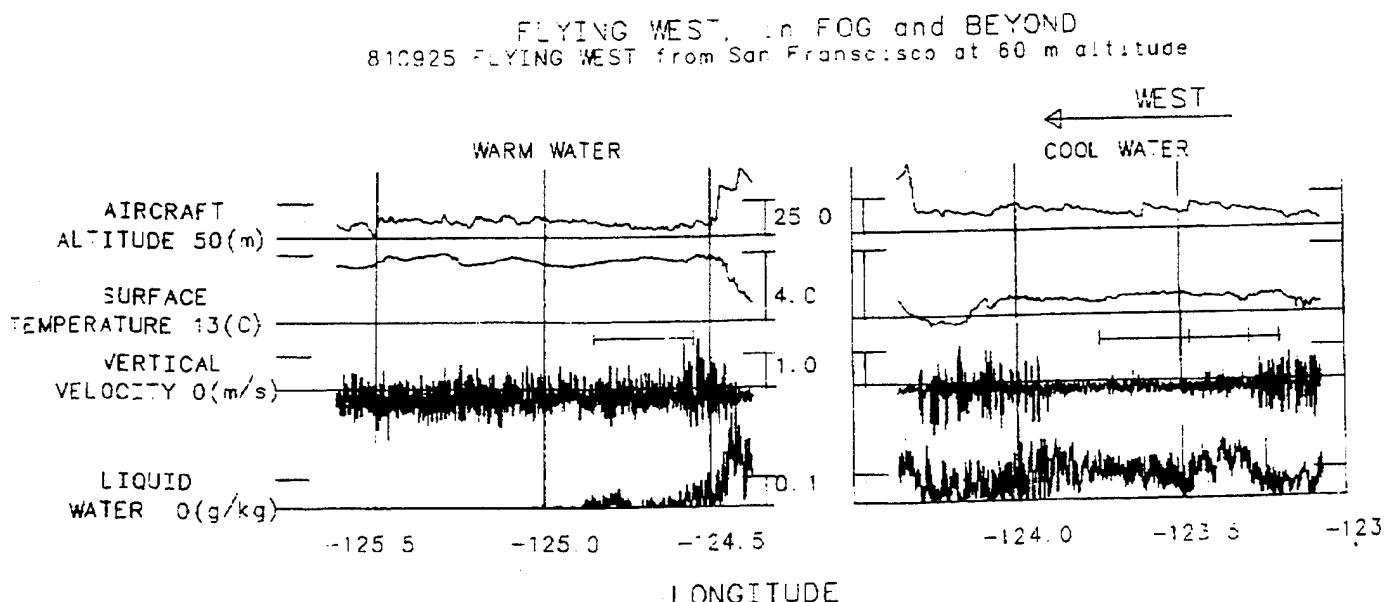


MARINE STRATUS  
CLOUD, LARGEST DROPS  
FROM PARCEL TO  
PARCEL

# FOG OBSERVATIONS



# **FOG IS COMPLETELY CALM**



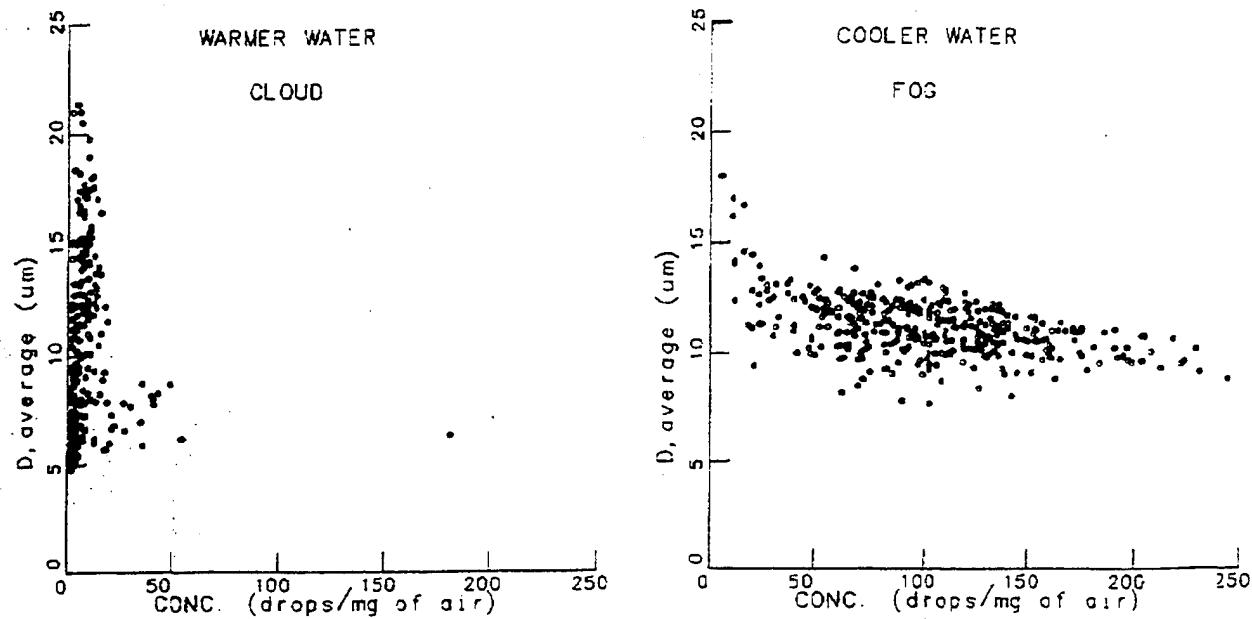
**FOG**

**THERE ARE NO DOWNDRAFTS  
IN THE FOG.**

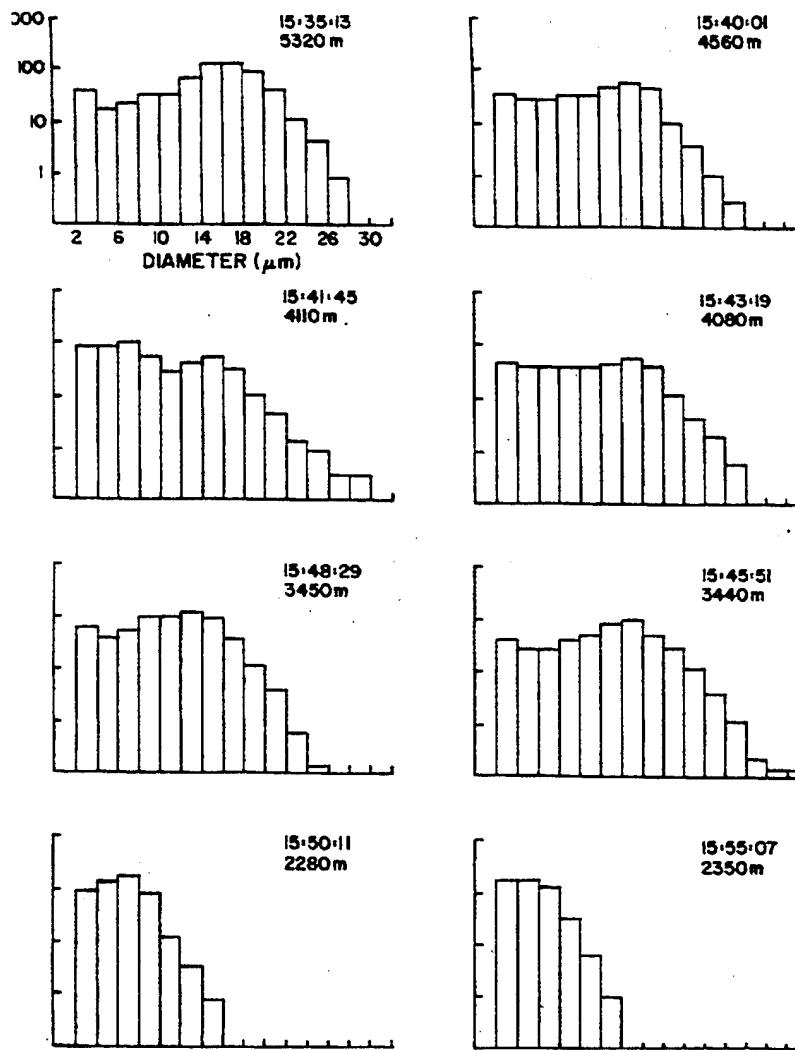
**HENCE THERE IS NO COOLING FLUX OF  
HEAT**

**HENCE THE FOG TOP IS NOT BEING  
COOLED BY RADIATION.**

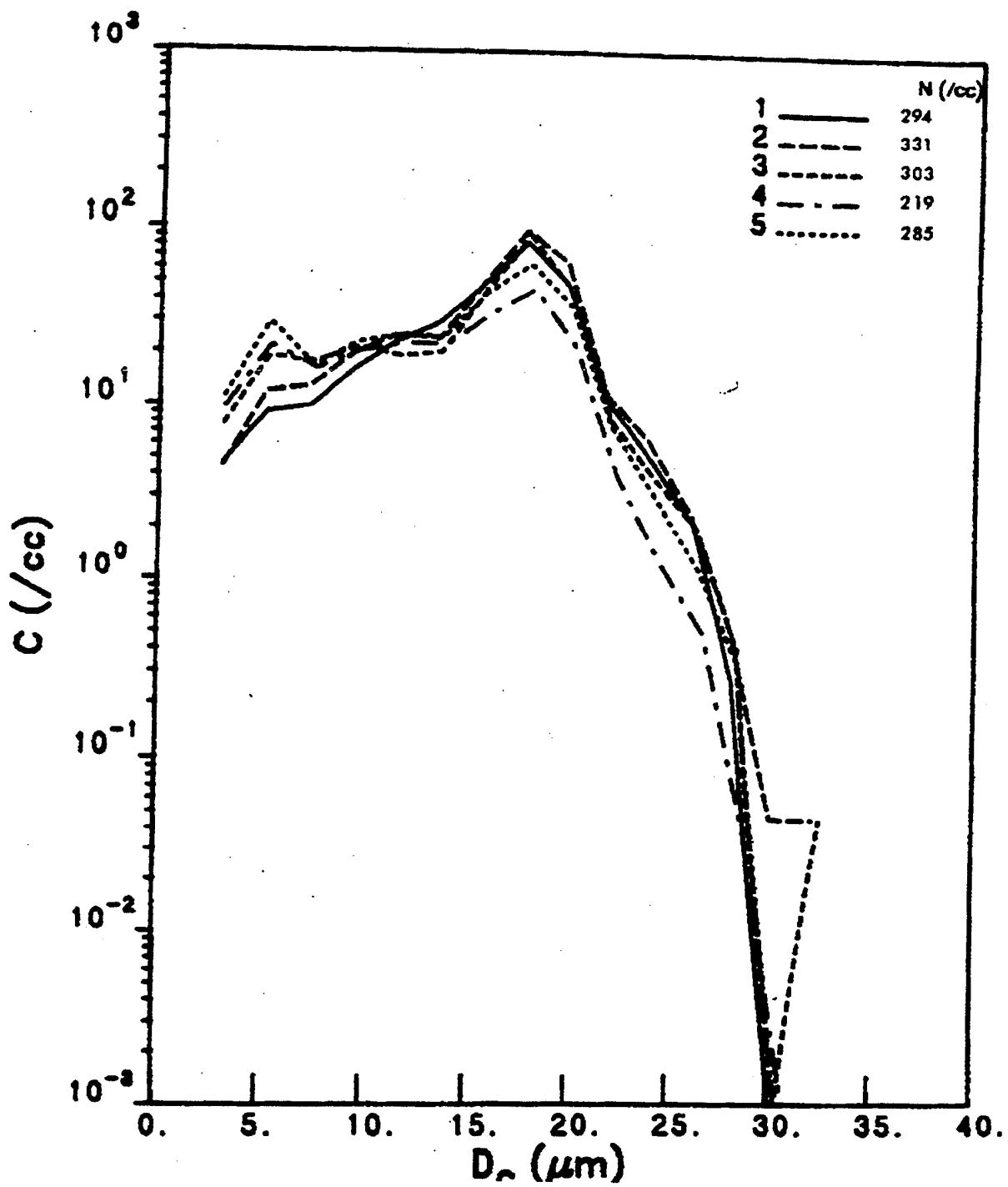
# **CONVECTING CLOUD      STILL FOG**



**ON THE RIGHT THE FOG DROPS AVERAGE ABOUT THE SAME DIAMETER ALTHOUGH THE CONCENTRATION VARIES BY 100 : 1**



## CLOUD DROP SPECTRA



## CLOUD DROP CHANGES AS CLOUD IS ENTERED



# SHARC-3: A Model for Infrared Atmospheric Radiance at High Altitudes

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R.D. Sharma, J.H. Brown, J.H. Gruninger, R.L. Sundberg,  
J.W. Duff, L.S. Bernstein, M.W. Matthew, S.M. Adler-  
Golden, D.C. Robertson, and R.J. Healey

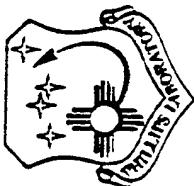
17th Annual Review Conference on Atmospheric  
Transmission Models

Phillips Laboratory  
Hanscom AFB

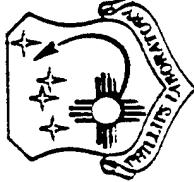
8 June 1994

# PRESENTATION OUTLINE

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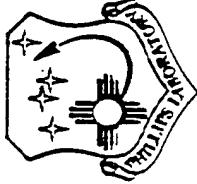
- OBJECTIVE
- SHARC OVERVIEW
- SHARC MODULES
  - AMBIENT POPULATIONS
  - AURORAL ENHANCEMENT
  - SPECTRAL RADIANCE
- SHARC-DATA COMPARISONS
  - SPIRE CO<sub>2</sub> EMISSION
  - SPIRE AND SPIRIT NO EMISSION
  - CIRRUS H<sub>2</sub>O AND O<sub>3</sub> EMISSION
- FUTURE PLANS
- SUMMARY



## SHARC OBJECTIVES

---

- COMPUTER CODE TO CALCULATE HIGH-ALTITUDE BACKGROUNDS IN QUIESCENT AND AURORALLY DISTURBED ATMOSPHERES
- PROVIDE SPECTRAL PREDICTIONS FOR RADIANCE AND TRANSMITTANCE ALONG ARBITRARY PATHS THROUGH THE ATMOSPHERE
  - MODEL ATMOSPHERIC EMISSION PROCESSES
  - SUPPORT AF MEASUREMENTS PROGRAMS CIRRIS 1A, SPIRIT II, MSX
  - PROVIDE CALCULATIONS FOR SYSTEMS STUDIES



# SHARC OVERVIEW

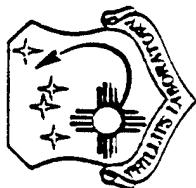
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- SHARC CALCULATES NLTE RADIATION FROM AMBIENT AND AURORAL ATMOSPHERES

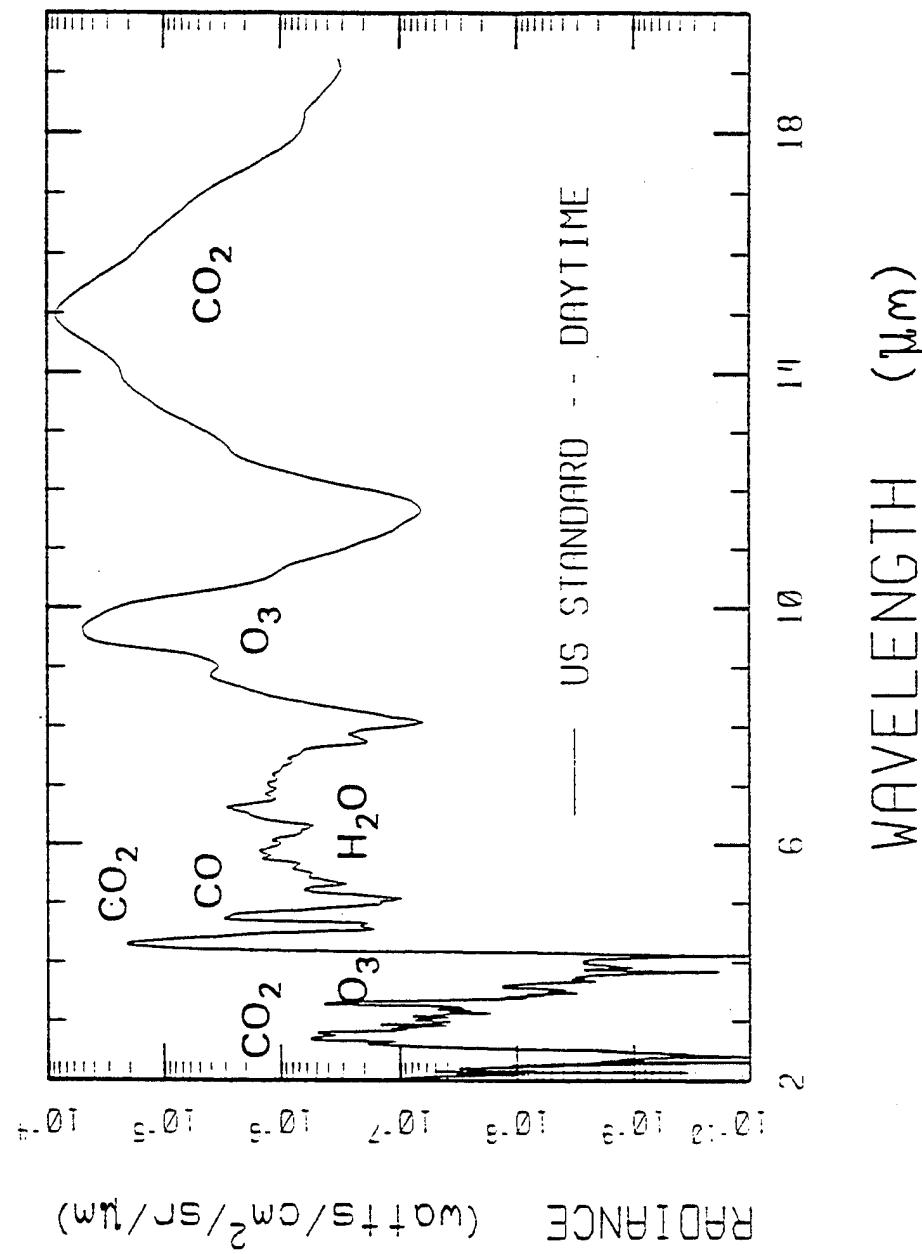
- SOME FEATURES:

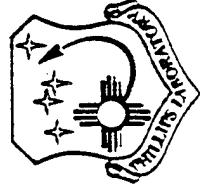
- 50-300 km ALTITUDE REGIME
- 2-40  $\mu\text{m}$  WITH A RESOLUTION OF  $0.5 \text{ cm}^{-1}$
- INTERACTIVE INPUT MODULE WITH ERROR CHECKING
- ADJUSTABLE CHEMICAL KINETICS MECHANISMS/RATES
- AUTOMATICALLY INCLUDES LTE & NLTE CONTRIBUTIONS
- AMBIENT MOLECULES INCLUDE:  $\text{H}_2\text{O}$ ,  $\text{O}_3$ ,  $\text{CO}$ ,  $\text{NO}$ ,  $\text{OH}$ ,  $\text{CO}_2$ , plus  $\text{H}_2\text{O}$  and  $\text{CO}_2$  ISOTOPES
- AURORAL MODULE WITH:  $\text{NO}^+$ ,  $\text{NO}$ ,  $\text{CO}_2$
- PATHS ACROSS AND AROUND THE SOLAR TERMINATOR

## ILLUSTRATIVE SHARC CALCULATION

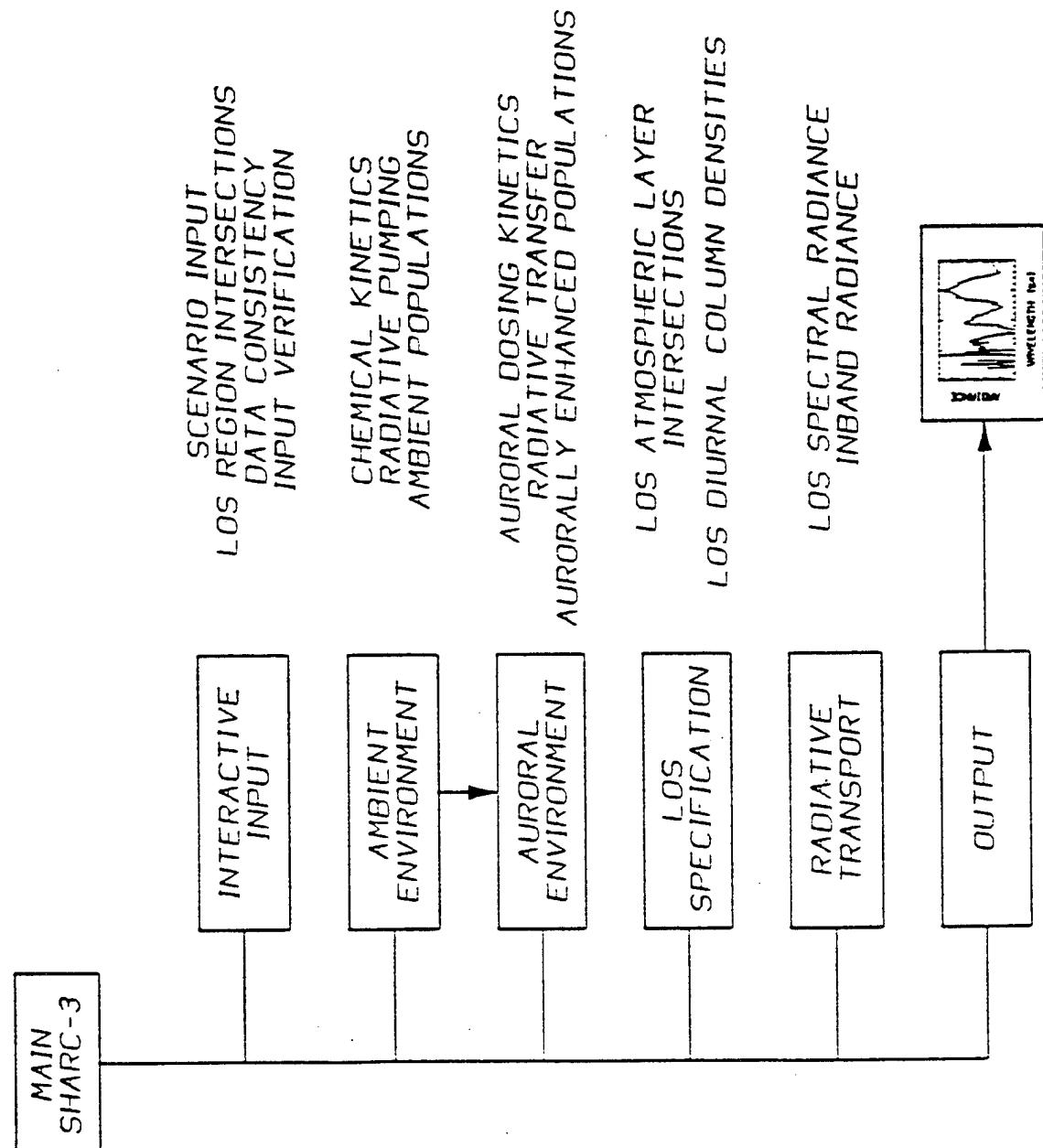


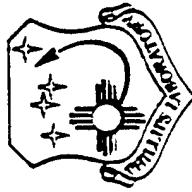
- SPACE VIEWING THROUGH A 50km LIMB PATH





# SHARC-3 FLOW CHART

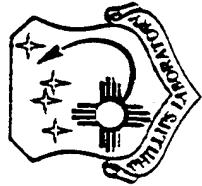




## AMBIENT POPULATIONS MODULE

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- SYMBOLIC DESCRIPTION OF CHEMICAL KINETICS
  - BASED ON WIDELY USED SANDIA CHEMKIN CODE
  - EXAMPLE:  
 $M + O + O_2 \rightarrow M + O_3(000)$   
 $M + O_3(001) \rightarrow M + O_3(000)$   
 $O_3(001) \rightarrow O_3(000) + h\nu$
- RATE EQUATIONS SOLVED IN STEADY STATE
- MONTE CARLO CALCULATION FOR RADIATIVE ENHANCEMENT
  - LAYER-LAYER PUMPING
  - IMPORTANT FOR THICK BANDS ( $CO_2$ )



## RADIATIVE EXCITATION MODULE (NEMESIS)

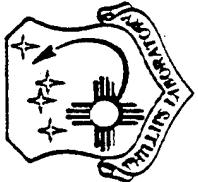
---

- RADIATIVE EXCITATION SIGNIFICANTLY ENHANCES EXCITED-STATE POPULATIONS OF STRONG BANDS AND HENCE THE STRENGTH OF THEIR EMISSIONS
- MONTE CARLO MODEL FOR LAYER-LAYER ABSORPTION AND EMISSION OF PHOTONS
- BASIC MODEL ASSUMPTIONS
  - SEMI-INFINITE PLANE-PARALLEL HOMOGENEOUS LAYERS
  - VOIGT LINESHAPE
  - TRANSLATIONAL-ROTATIONAL EQUILIBRIUM
  - COMPLETE LINE FREQUENCY REDISTRIBUTION
  - COMPLETE ROTATIONAL LEVEL REDISTRIBUTION
  - NO LINE OVERLAP



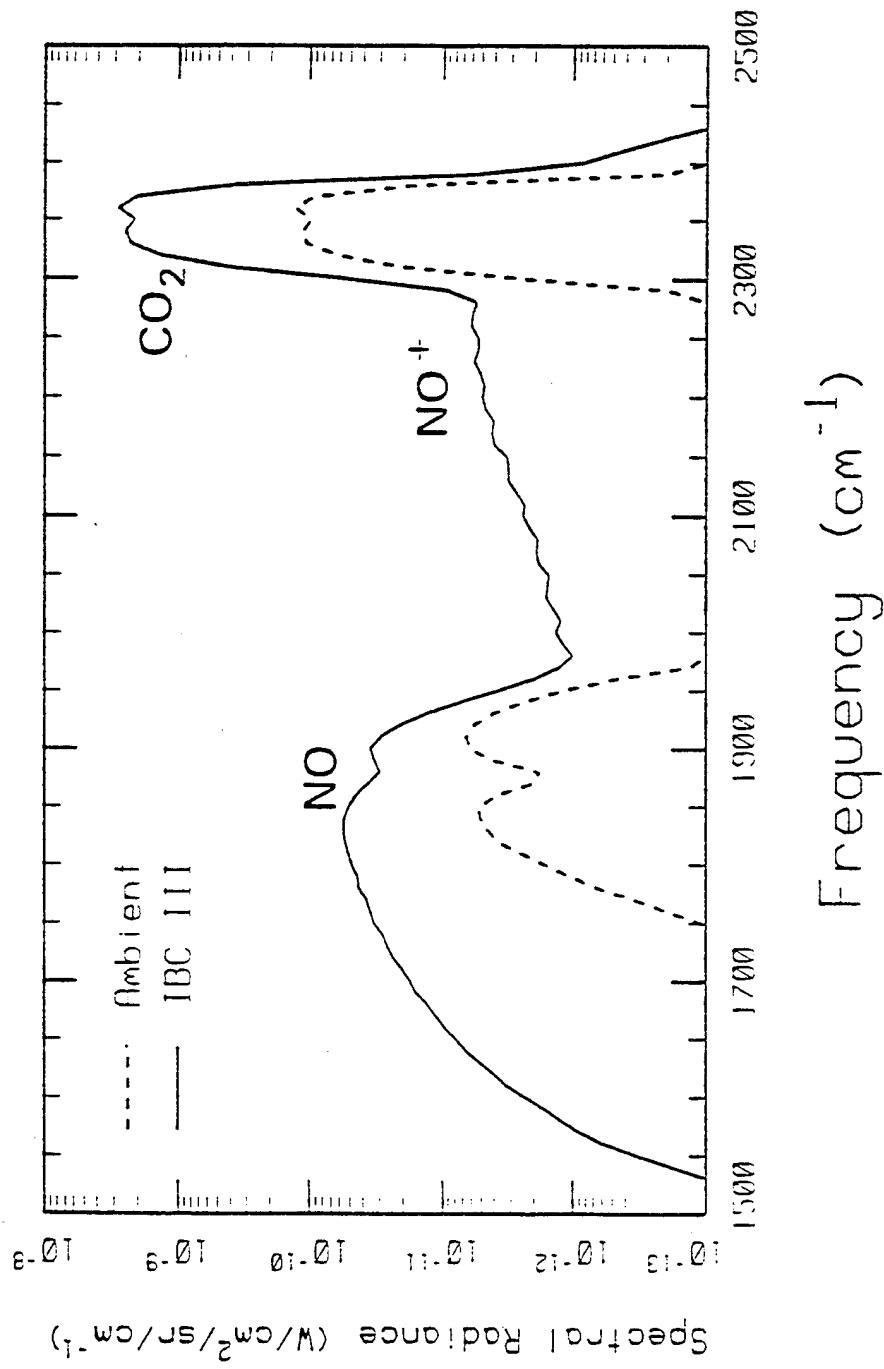
## SHARC AURORAL MODULE

- AURORAL PHENOMENOLOGY
  - ELECTRON DEPOSITION MODELS FOR DIFFERENT STRENGTH AURORAS: CLASS II, III, III+
  - SOLVES TIME/ENERGY DEPENDENT RATE EQUATIONS TO CALCULATE BOTH SECONDARY ELECTRON DISTRIBUTIONS AND THE KINETICS FOR IR RADIATORS
  - CALCULATES PRODUCTION OF ATMOSPHERIC NO and NO<sup>+</sup>
  - PRESENT IR MOLECULES ARE: NO, NO<sup>+</sup>, CO<sub>2</sub>
- SHARC AURORAL APPROACH
  - GEAR'S STIFF ODE ALGORITHM USED
  - CAN ADD NEW RADIATORS VIA USER-DEFINED INPUT FILES
  - LOCALIZED AURORAL REGION(S) EMBEDDED IN AMBIENT ATMOSPHERE
- GEOMETRY MODEL INSURES THAT LOS TRAJECTORIES INTERSECT AURORA AS DESIRED



## ILLUSTRATIVE AURORAL ENHANCEMENT

- PATH 90 km - SPACE





## COMPARISON TO AURORAL FIELD DATA

### • FWI DATA (FIELD WIDENED INTERFEROMETER)

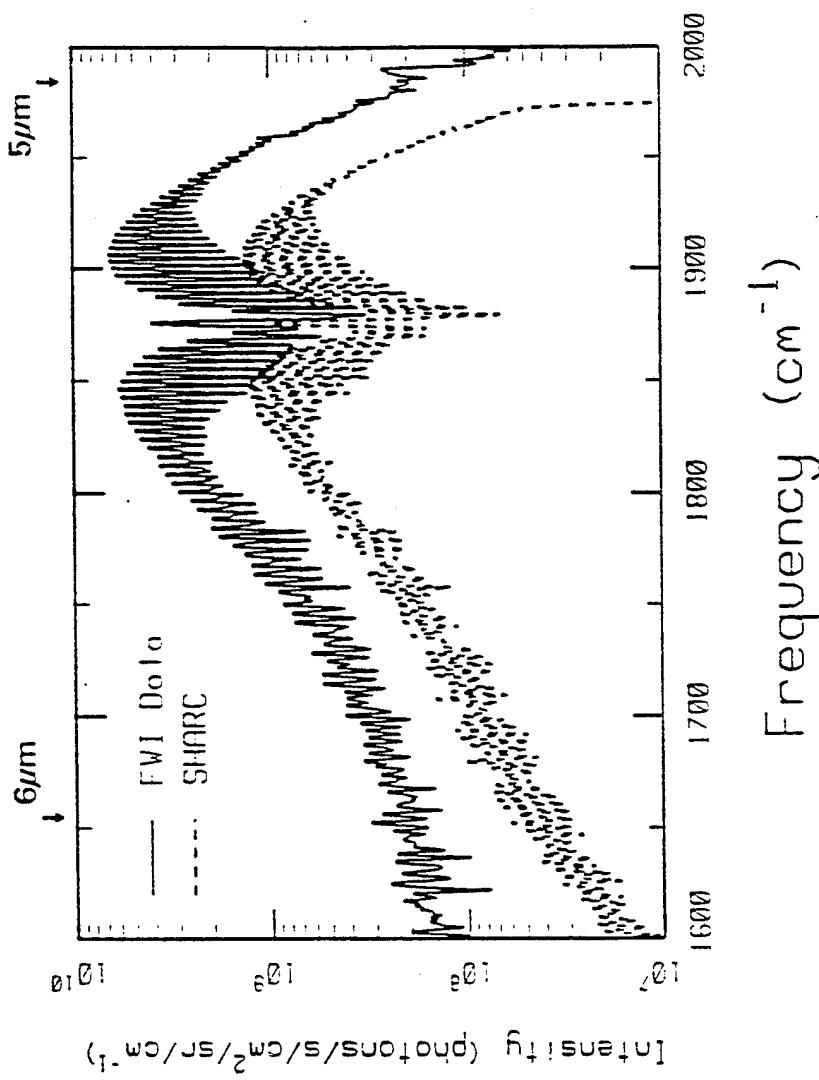
- VERTICAL PATH  
90 KM TO SPACE

- CLASS II AURORA

- $N(^2D) + O_2$  REACTION  
TO PRODUCE NO<sup>\*</sup>

**BUT**

- CURRENT WORK  
SUGGESTS N(<sup>4</sup>S)  
IMPORTANT TOO





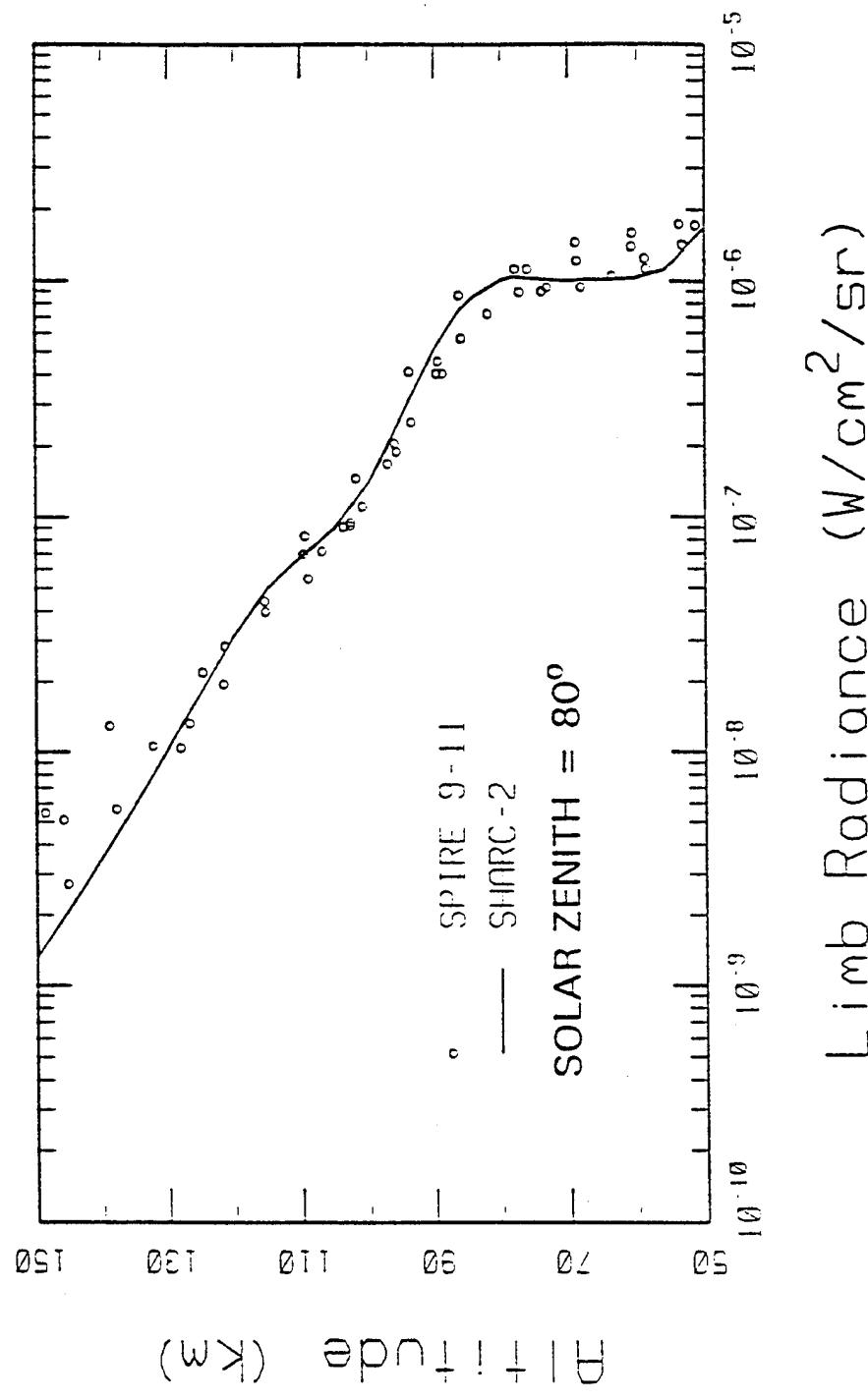
## SPECTRAL RADIANCE MODULE

- RADIATION TRANSPORT CALCULATION PERFORMED FOR  
EACH MOLECULAR LINE
  - USES PL ATMOSPHERIC ABSORPTION LINE DATABASE (HITRAN)
- RODGERS-WILLIAMS APPROXIMATION FOR VOIGT EQUIVALENT  
WIDTH OF A SINGLE LINE
- LAYER-DEPENDENT LINE STRENGTHS
- CURTIS-GODSON APPROXIMATION
  - AVERAGING PROCEDURE FOR INHOMOGENEOUS PATHS
- LINE OVERLAP CORRECTION FOR DENSE REGIONS
- 50-70 TIMES FASTER THAN TRADITIONAL LBL APPROACH

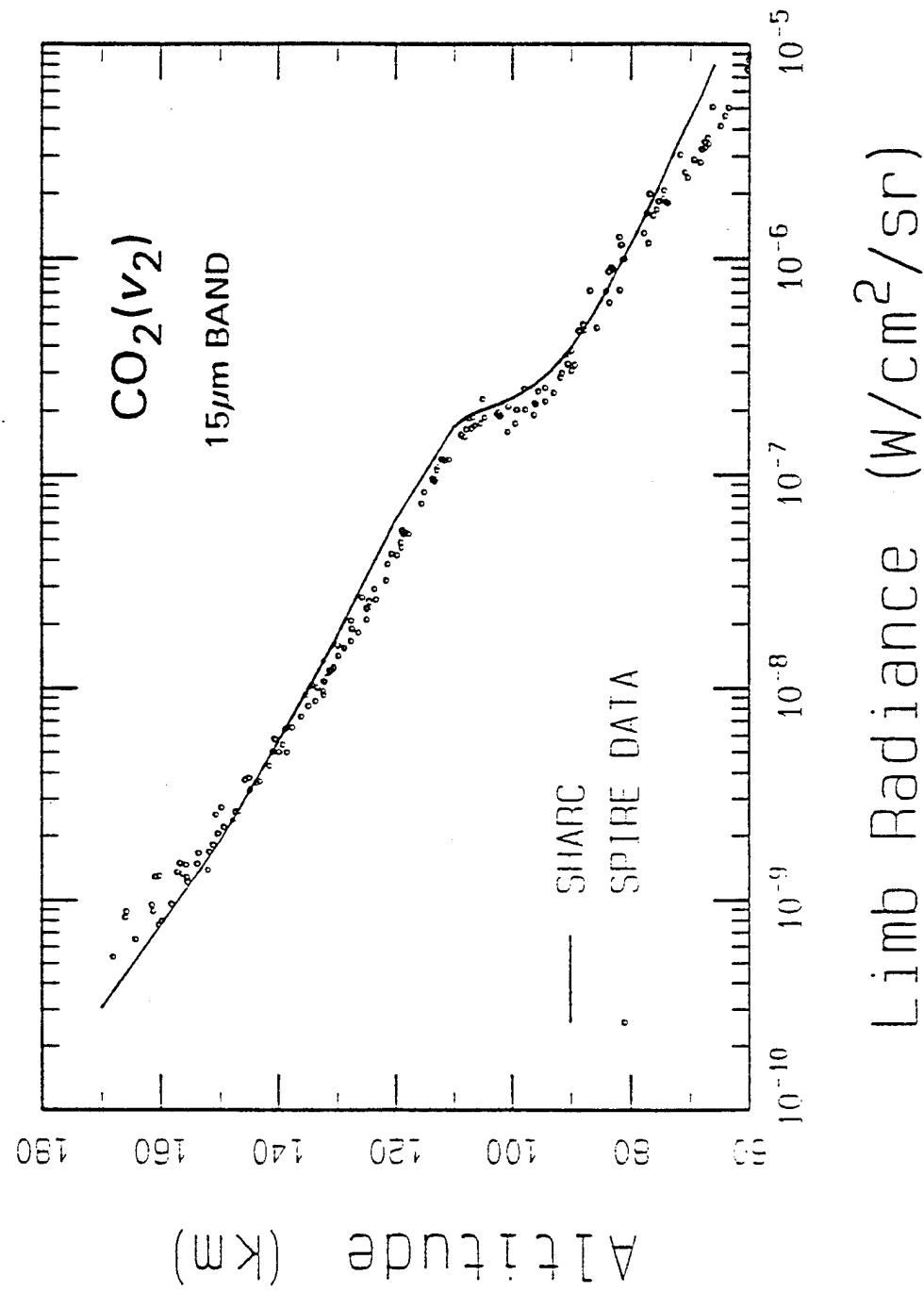
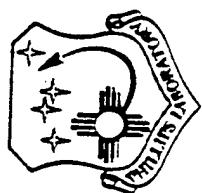


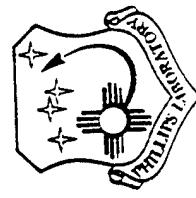
## SPIRE: DAYTIME CO<sub>2</sub> (4.3 $\mu\text{m}$ )

- SOLAR PUMPED VIA EXCITATION OF SHORT WAVE IR BANDS



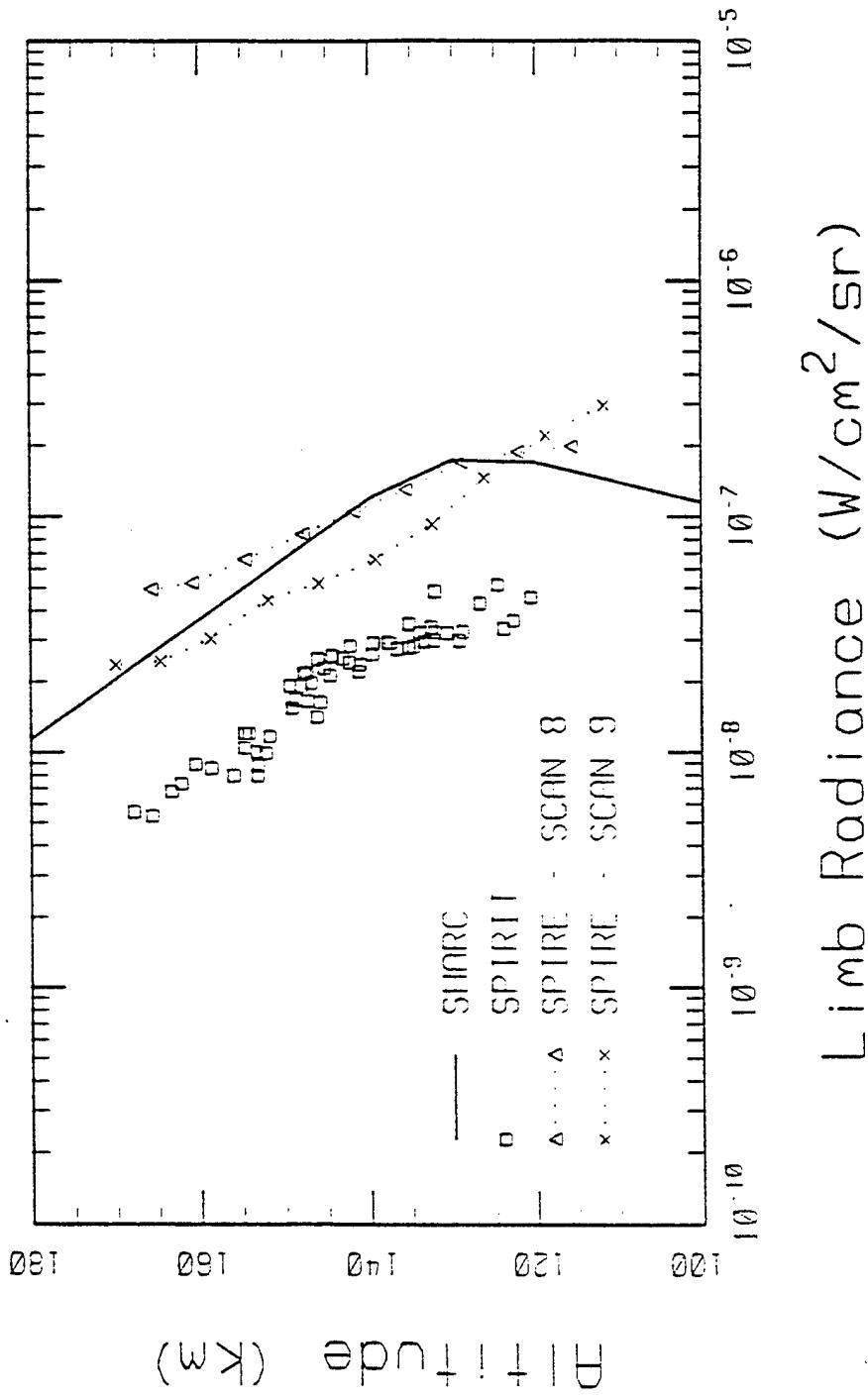
# SPIRE: LONG WAVE CO<sub>2</sub>

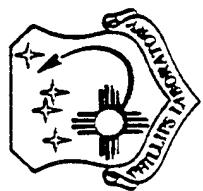




## COMPARISON TO NO (5.3 $\mu\text{m}$ ) DATA

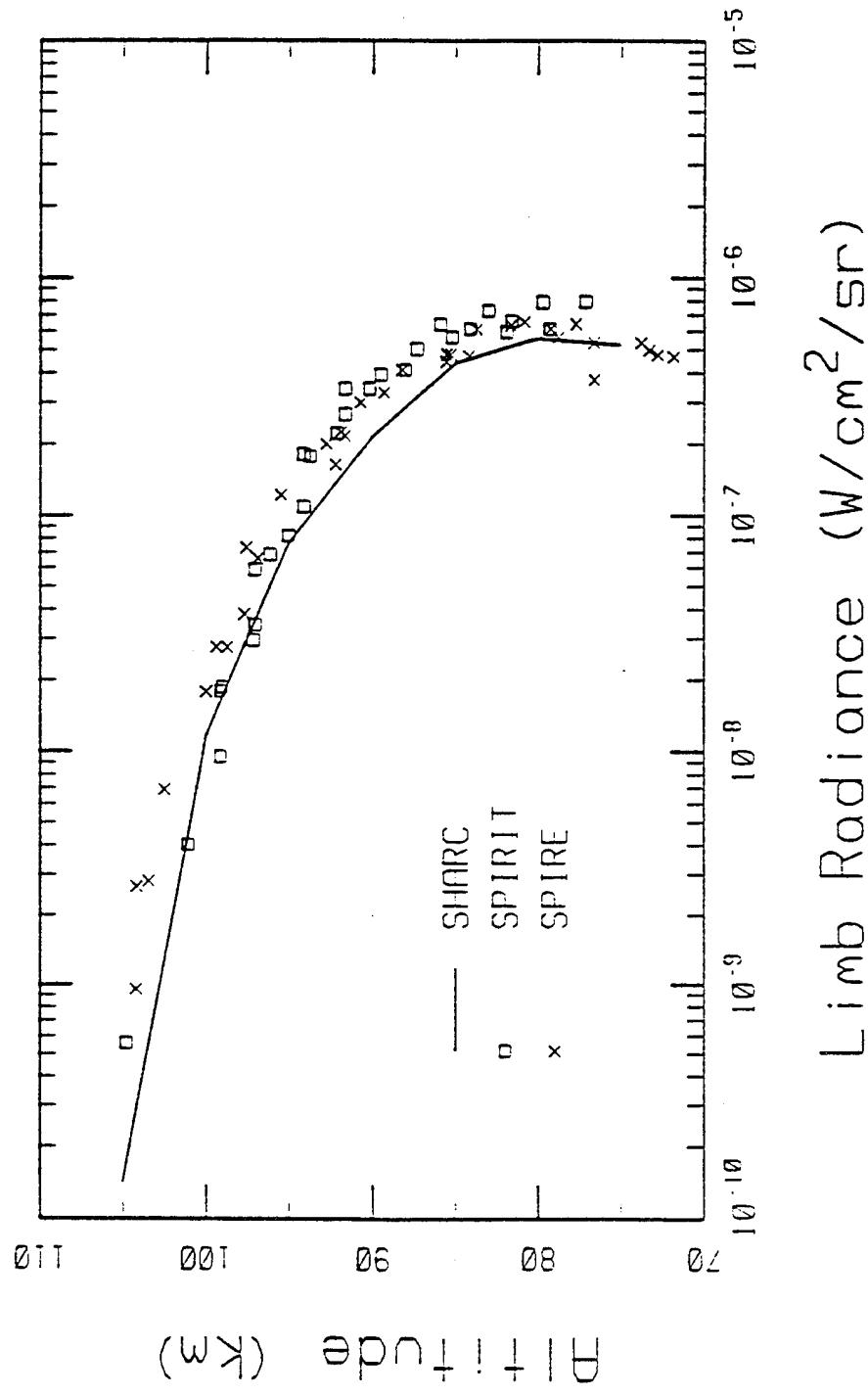
- SIGNIFICANT VARIABILITY IN OBSERVED NO RADIANCES



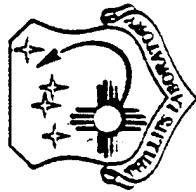


## COMPARISON TO O<sub>3</sub>(9.6 $\mu$ m) DATA

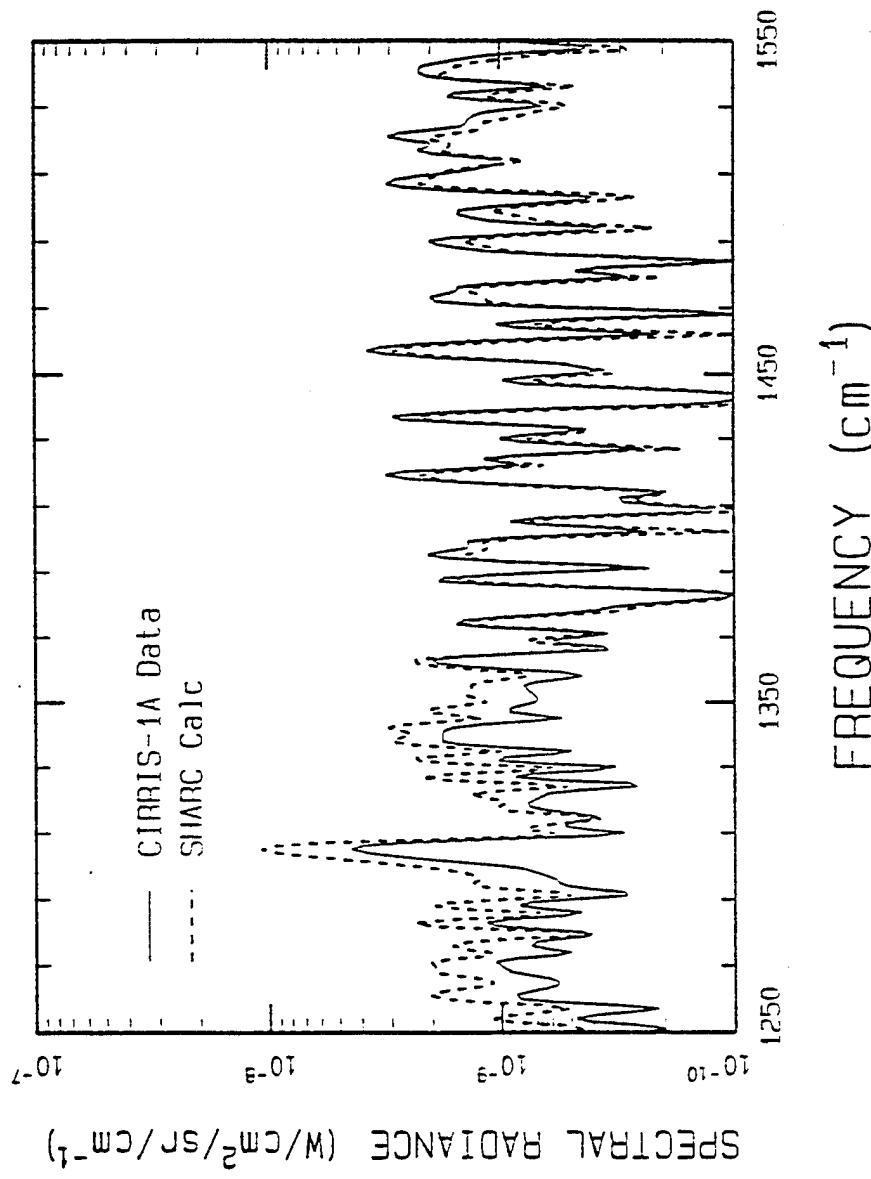
- SPIRIT 1 AND SPIRE DATA FOR NIGHTTIME CONDITIONS

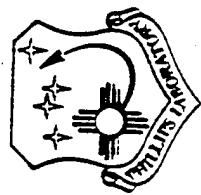


## COMPARISON TO CIRRIS DATA



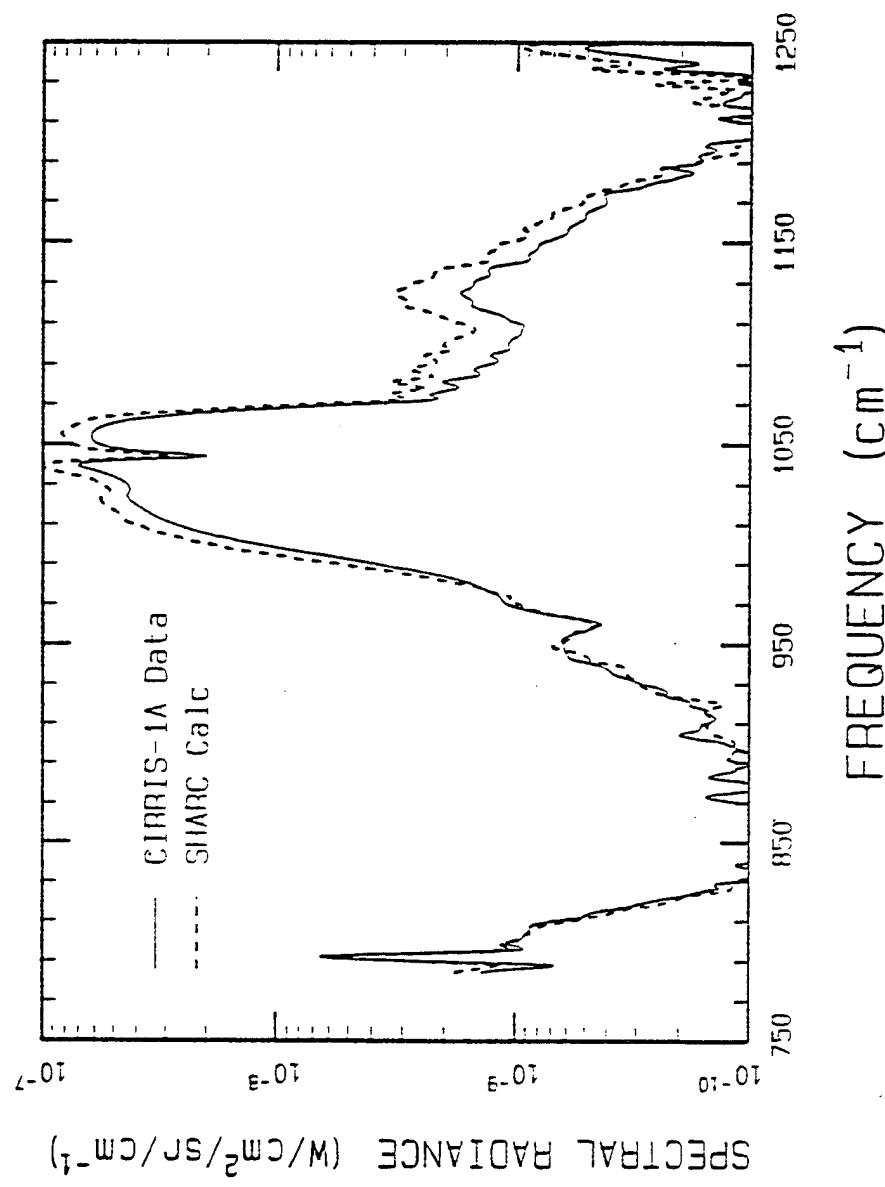
### • ILLUSTRATIVE CIRRIS SPECTRAL DATA FOR LIMB VIEWING





## COMPARISON TO CIRRIS DATA (cont.)

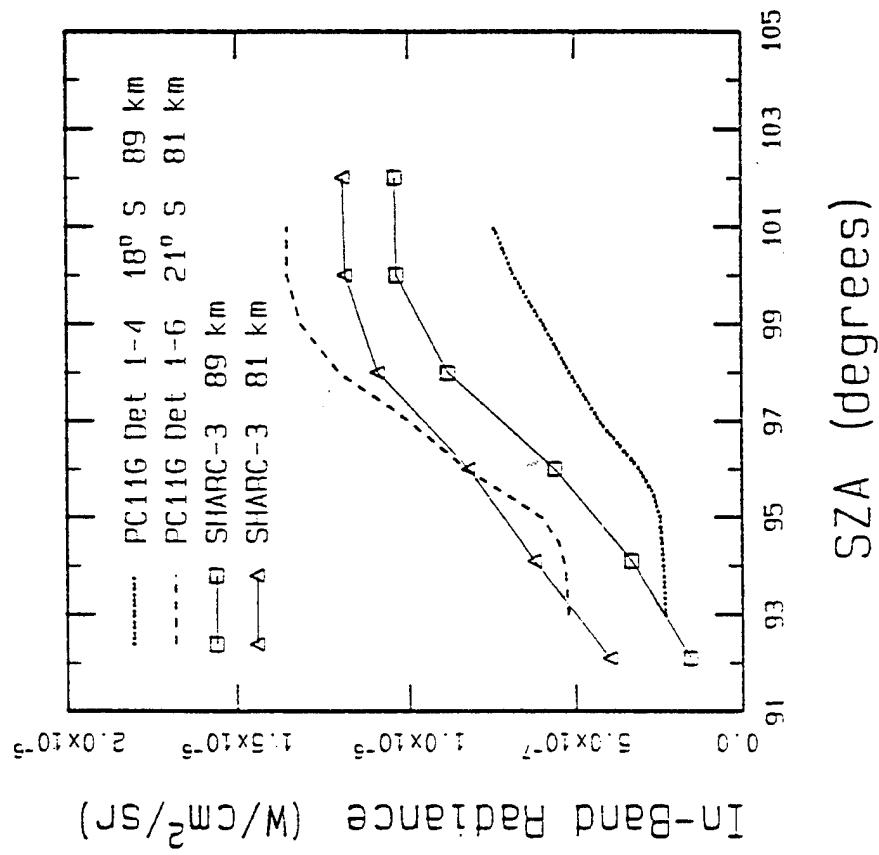
### • ILLUSTRATIVE CIRRIS SPECTRAL DATA FOR LIMB VIEWING





# LIMB VIEWS ALONG SOLAR TERMINATOR

- CIRRIS IN-BAND DATA FOR LIMB VIEWS

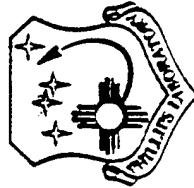


# RUN TIMES - CHEMISTRY

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- CHEMISTRY REPEATED ONLY FOR MODIFIED ATMOSPHERE
- AMBIENT POPULATIONS
  - 89 BANDS OF H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, CO, NO, OH
    - 26 OF WHICH REQUIRE RADIATION TRAPPING TREATMENT
  - 66 ATMOSPHERIC LAYERS FROM 50 TO 300 KM
- DATA GENERAL AVIION AV5100 (20 MIPS) : 15.2 MIN  
DEC VAX 8800 : 10.8 "  
DEC VAX 780 : 80.1 "
- AUORAL POPULATIONS (ADDITIONAL TO AMBIENT)
  - 31 VIBRATIONAL STATES: NO(13), NO<sup>+</sup>(14), CO<sub>2</sub>(4)
  - 37 RADIATING BANDS: NO(23), NO<sup>+</sup>(13), CO<sub>2</sub>(1)
  - 36 LAYERS FROM 80 TO 150 KM
- DATA GENERAL AVIION AV5100 (20 MIPS) : 7-12 MIN  
DEC VAX 8800 : 5- 8.5 "  
DEC VAX 780 : 37-64 "



## RUN TIMES - LOS RADIANCE

---

- SPECTRAL RADIANCE - SINGLE BAND

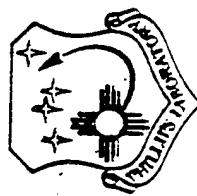
- 14-16  $\mu\text{m}$  BAND OF CO<sub>2</sub> WITH 890 LINES
- 131 LAYERS (50 KM LIMB)

DATA GENERAL AViiON AV5100 (20 MIPS): 5.2 SEC  
DEC VAX 8800 : 3.7 "  
DEC VAX 780 : 27.6 "

- SPECTRAL RADIANCE - MULTIPLE BANDS

- 1-40  $\mu\text{m}$  BANDPASS: H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, CO, NO, OH  
84,000 LINES
- 131 LAYERS (50 KM LIMB)

DATA GENERAL AViiON AV5100 (20 MIPS): 6.3 MIN  
DEC VAX 8800 : 4.5 "  
DEC VAX 780 : 33.4 "



## FUTURE PLANS

---

- VALIDATION AND UPGRADES BY COMPARISON TO  
THE CIRRIS-1A DATA BASE
- DEVELOPING MODULE FOR ATMOSPHERIC STRUCTURES
  - SPECTRAL-SPATIAL CLUTTER METRICS
  - SPIE PAPER 2223-26
- INTERFACED SHARC WITH THE LOW-ALTITUDE CODE
  - SAMM: SHARC AND MODTRAN MERGED
- EXTEND INTO THE NEAR INFRARED AND VISIBLE  
SPECTRAL REGIONS



## SUMMARY

---

- SHARC IS A HIGH-ALTITUDE RADIANCE MODEL FOR  
THE INFRARED SPECTRAL REGION
  - AURORAL AND QUIESCENT ATMOSPHERES
  - DIURNAL VARIATION INCLUDING SOLAR TERMINATOR
  - MODULARIZED STRUCTURE
  - ARBITRARY PATHS ABOVE 50 km
  - LINE-BY-LINE RADIANCE CALCULATIONS
  - FULLY INTEGRATED & LOCALIZED AURORAL REGION(S)
  - CLUTTER MODULE UNDER DEVELOPMENT
  
- VALIDATED WITH FIELD DATA TAKEN BY THE  
GEOPHYSICS DIRECTORATE, PHILLIPS LABORATORY
  - CIRRIS, SPIRE, SPIRITS, FWI, etc.

# Non-LTE in CO<sub>2</sub> in the middle atmosphere

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## 1 Introduction

- LTE
- vib. non-LTE and rot. LTE
- total non-LTE

Techniques used to model  
non-LTE

- Lambda iteration ( $L \times L$ )
- Curtis-matrix tech. ( $L \times D \times L = D$ )
- ALI tech. ( $L \times L$ )

## **2 System of vibrational energy levels and radiative transitions of CO<sub>2</sub>**

We considered *all* vibrational levels and *all* ro-vibrational lines for the C<sup>12</sup>O<sub>2</sub><sup>16</sup> isotope which are available from HITRAN-92: the excitation of  $\nu_2$ - and  $\nu_3$ - vibrations up to  $5\nu_2$  and  $3\nu_3$  respectively.

Radiative processes: (a) absorption of direct solar radiation and the radiation coming from the lower boundary, (b) absorption of atmospheric radiation and (c) spontaneous and stimulated emission.

### **Quantitative characteristics of the model:**

Total number of vibrational levels:  $L_v=127$

Total number of ro-vibrational levels:  $L=7499$

Total number of bands: 324

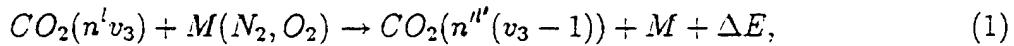
Total number of ro-vibrational lines: 29993

## 2.1 Collisional processes

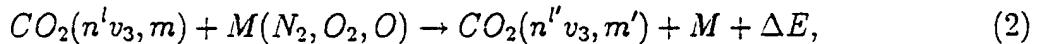
### 2.1.1 R-T processes

Assumption of rotational LTE (infinite large rate of the R-T exchange)

### 2.1.2 Intra-molecular V-V processes

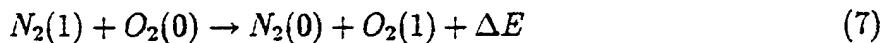
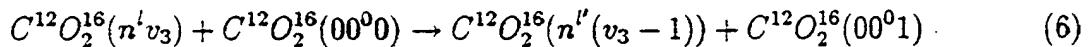
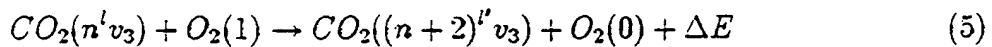
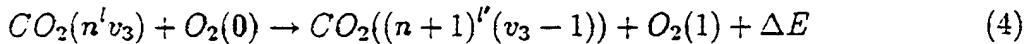
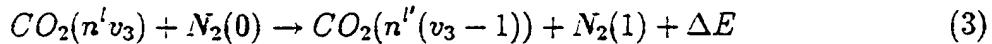


where  $n' = n + 1, n + 2, n + 3, n + 4$ .

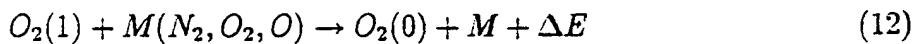
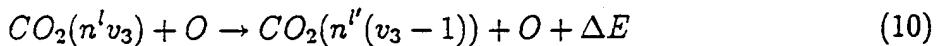
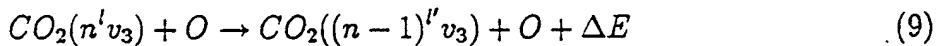
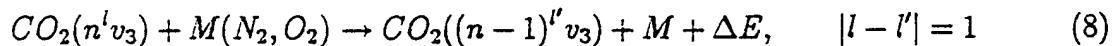


where  $m$  and  $m'$  denote arbitrary levels from the groups  $n^l v_3$  and  $n'' v_3$  respectively.

### 2.1.3 Inter-molecular V-V processes



### 2.1.4 V-T processes



## **2.2 Reference atmosphere**

Temperature profiles, mixing ratio profiles for N<sub>2</sub>, O<sub>2</sub> and O: MSISE-90 reference atmosphere.

The volume mixing ratio for CO<sub>2</sub> was compiled on the basis of experimental data, presented by Trinks and Fricke (1978), Offermann et al (1981) and Rinland et al (1992).

## **2.3 Computational features**

On each iteration step we solve the radiative transfer equation in each of 29993 ro-vibrational lines using the Feautrier technique for 16 frequency and 4 angle grid points.

In order to reach the convergence criterion  $10^{-4}$  for vibrational populations 6 and 40 accelerated lambda iterations are required for day and night conditions respectively.

## 2.4 Results

### 2.4.1 Verification of standard approximations

1. Effect of highly excited levels

2."Emission" and "radiative temperature" approximations for weak bands

3. Spontaneous emission

$$\sum_j n_{vj} A_{vj,v'j'} = n_v \sum_j W_v^{LTE}(j, T) A_{vj,v'j'} = n_v A_{v,v'}(T) \quad (13)$$

where

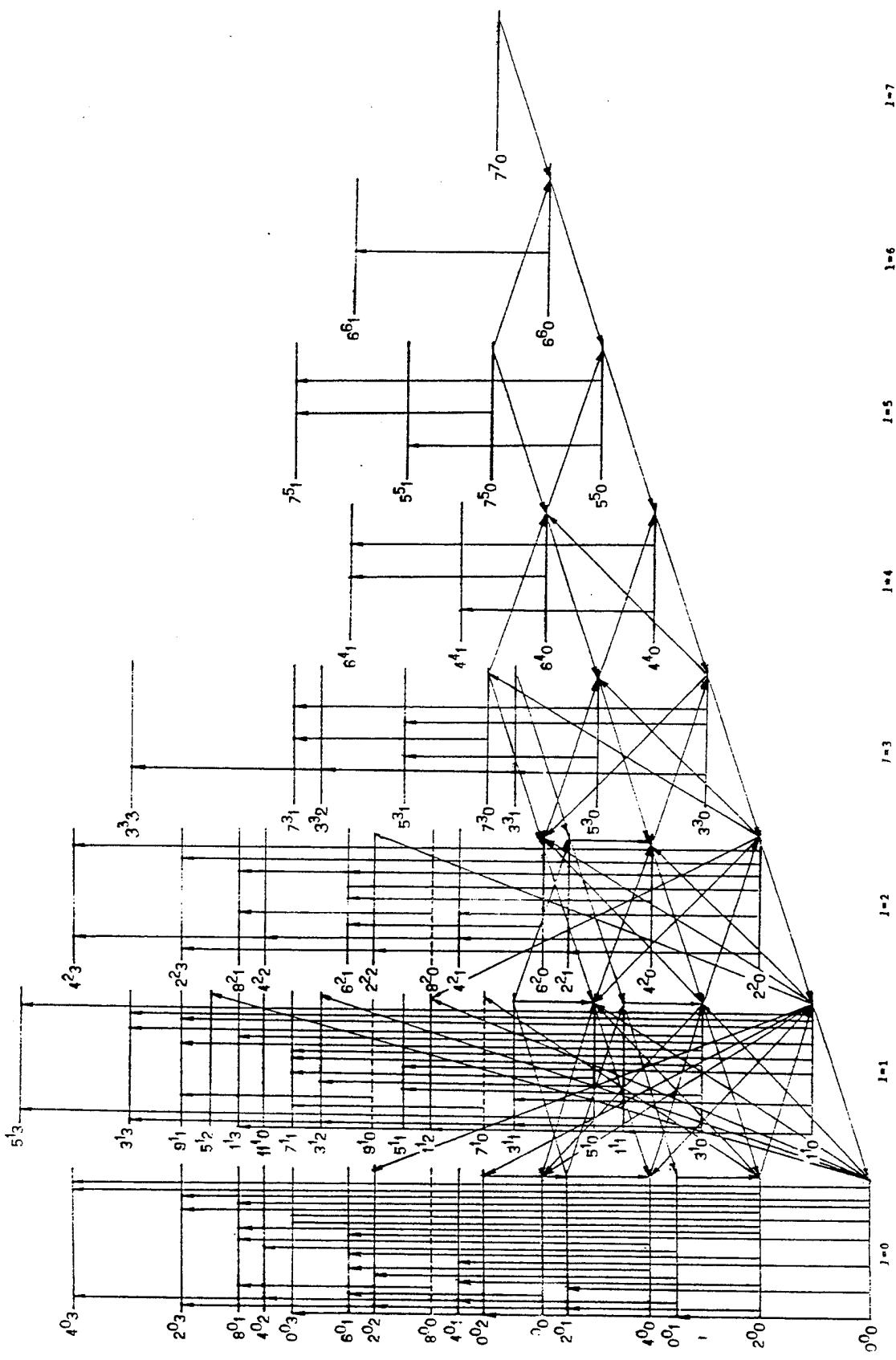
$$W_v^{LTE}(j, T) = \frac{g_v(j) \exp(-\frac{E_v(j)}{k_B T})}{Q_v(T)} \quad (14)$$

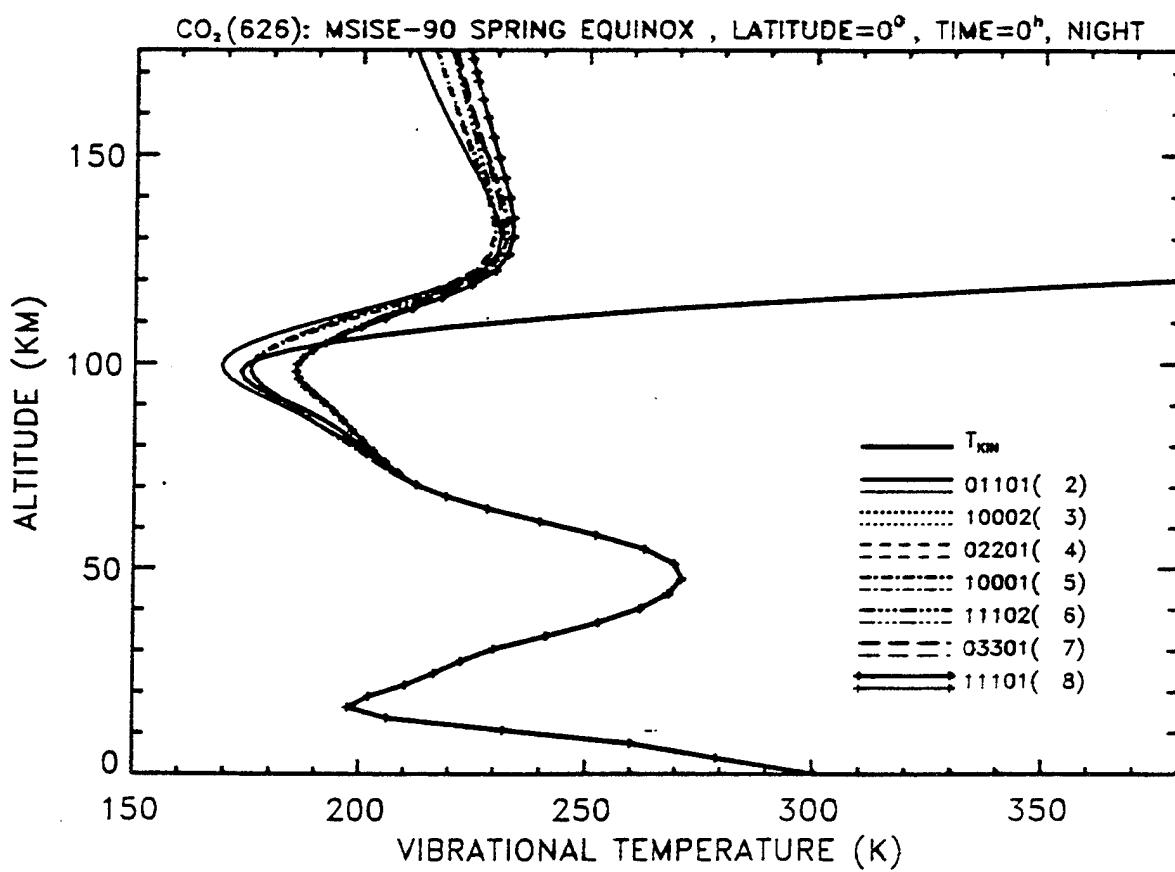
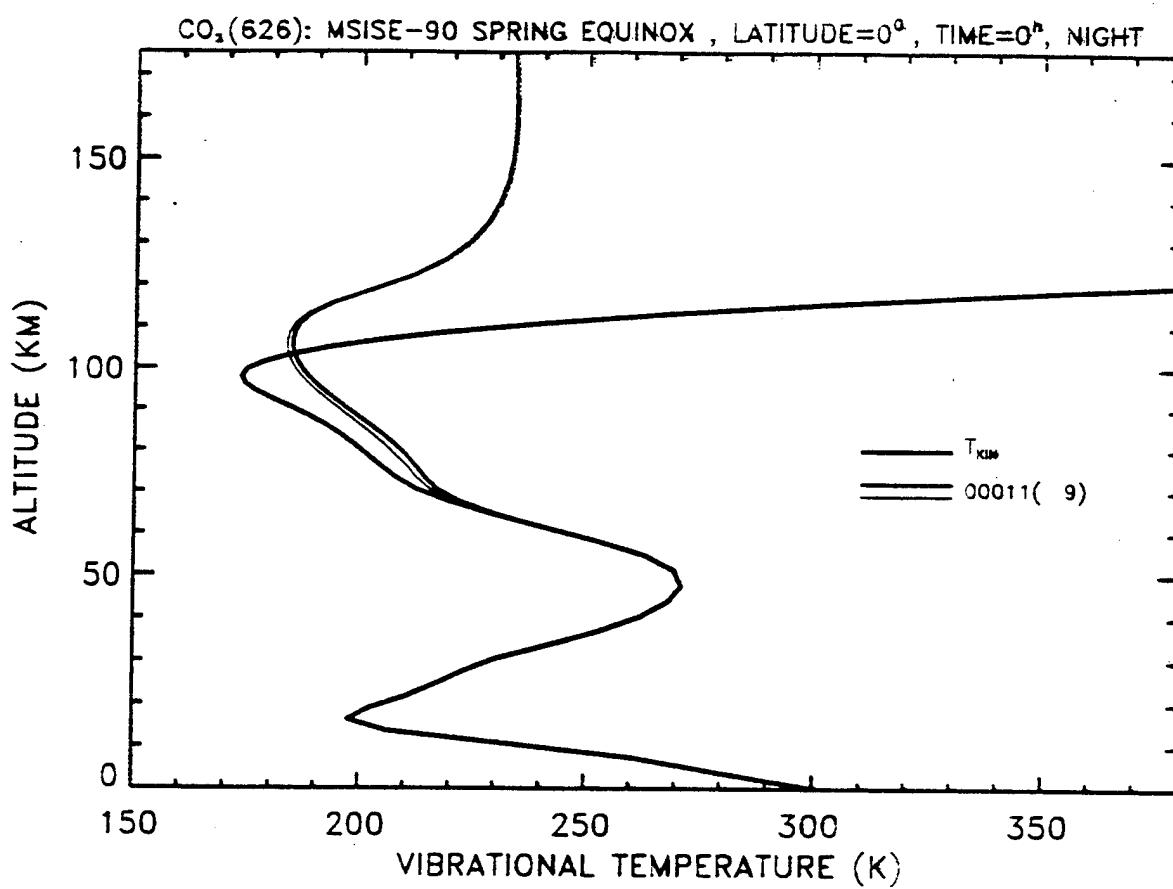
4. Weak transitions, not presented in HITRAN-92

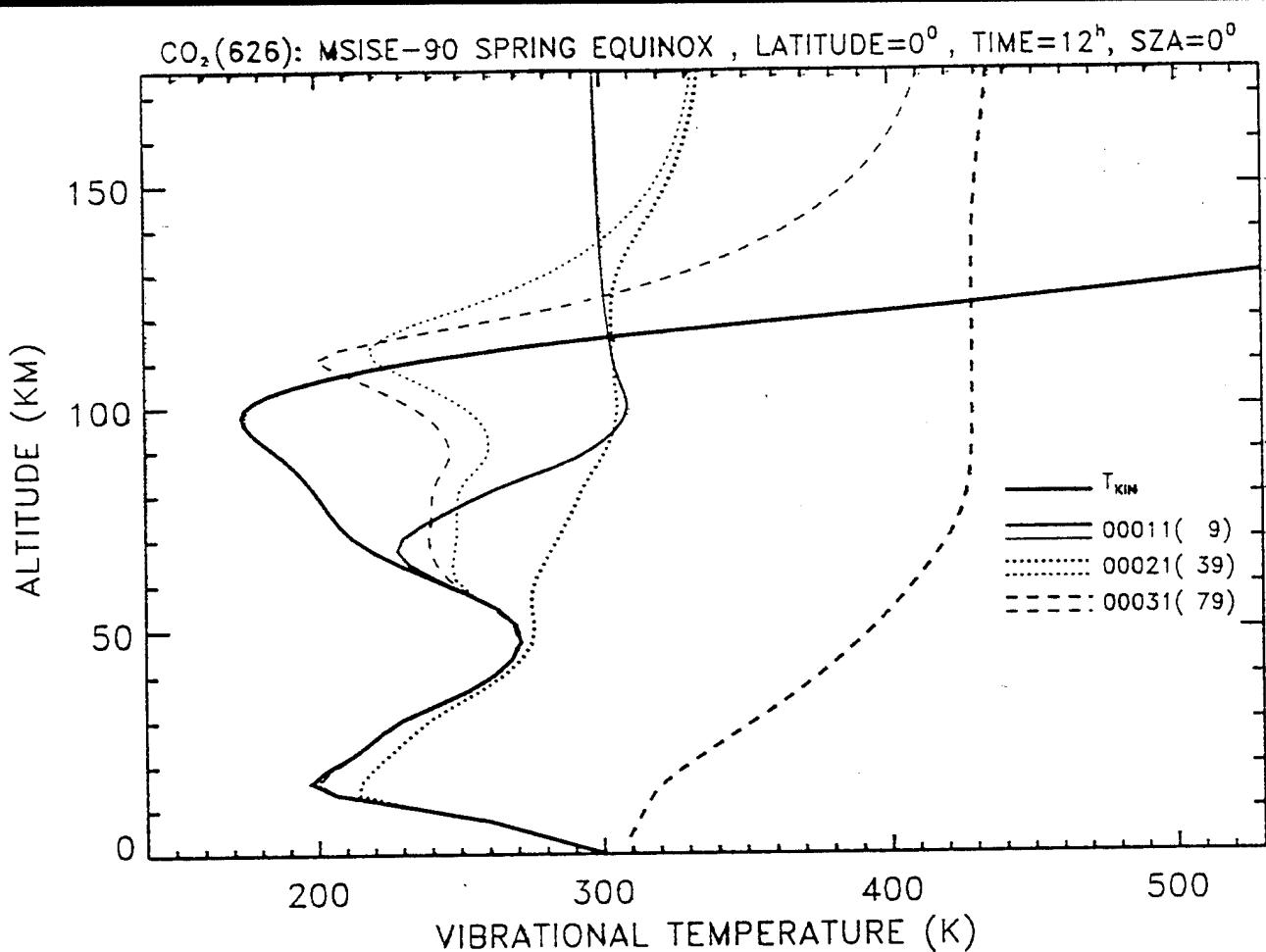
5. Laser transitions around  $10\mu\text{m}$

### 2.4.2 Influence of collisional rate coefficients

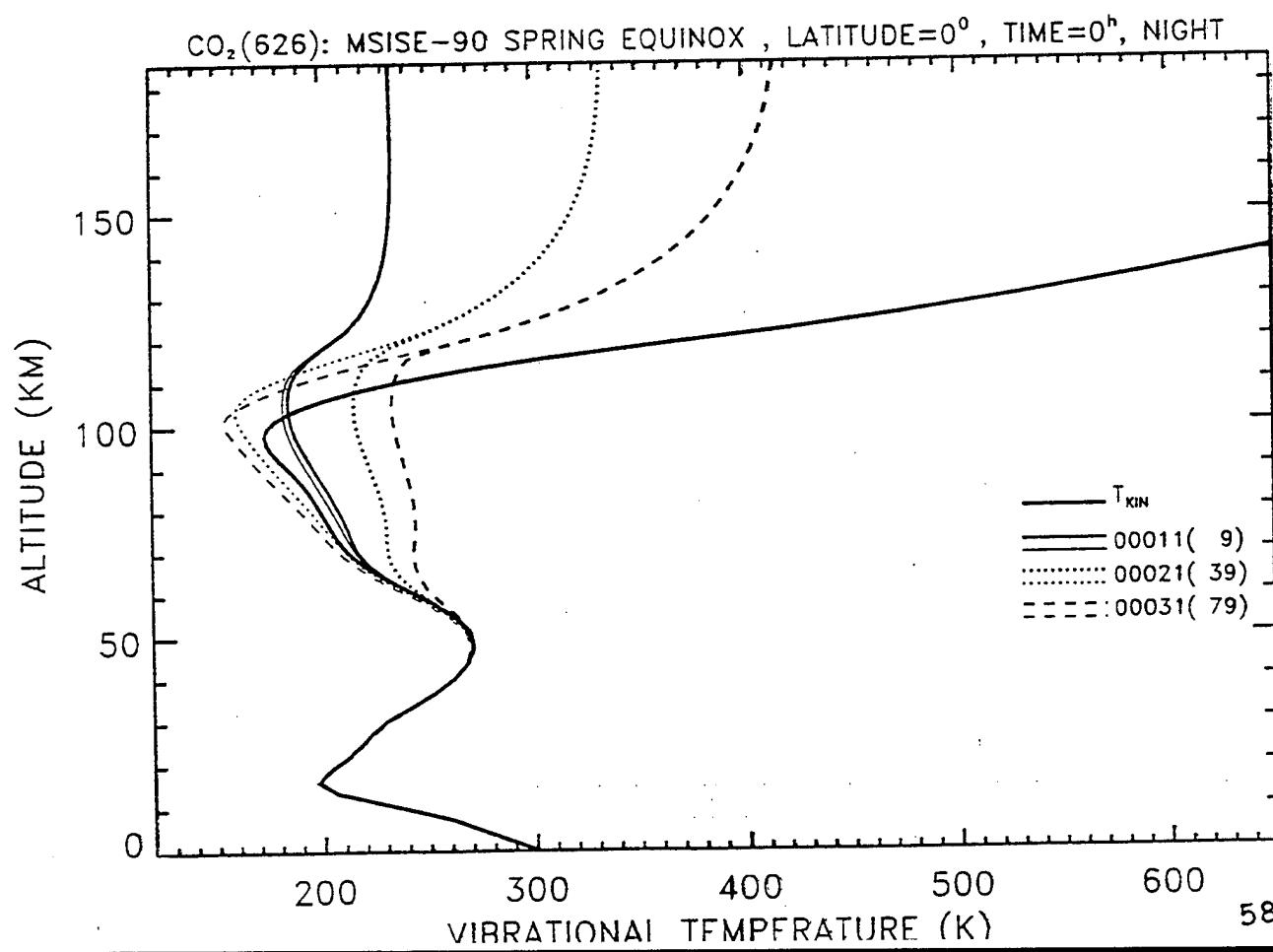
- Rate coefficient for quenching of the  $\nu_2$  transitions by atomic oxygen: 1.5, 3 and  $6 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$ .
- Multi-quantum and one-quantum quenching of vibrations by atomic oxygen

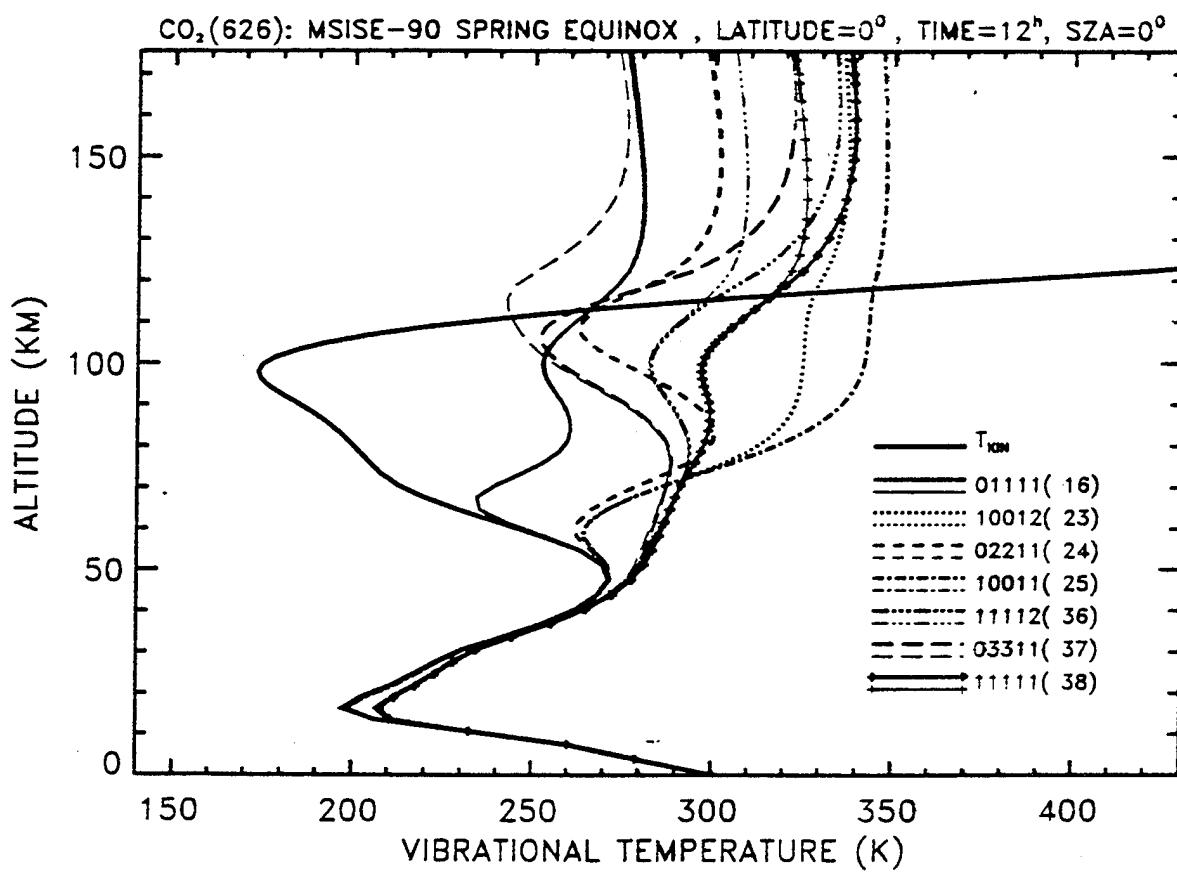
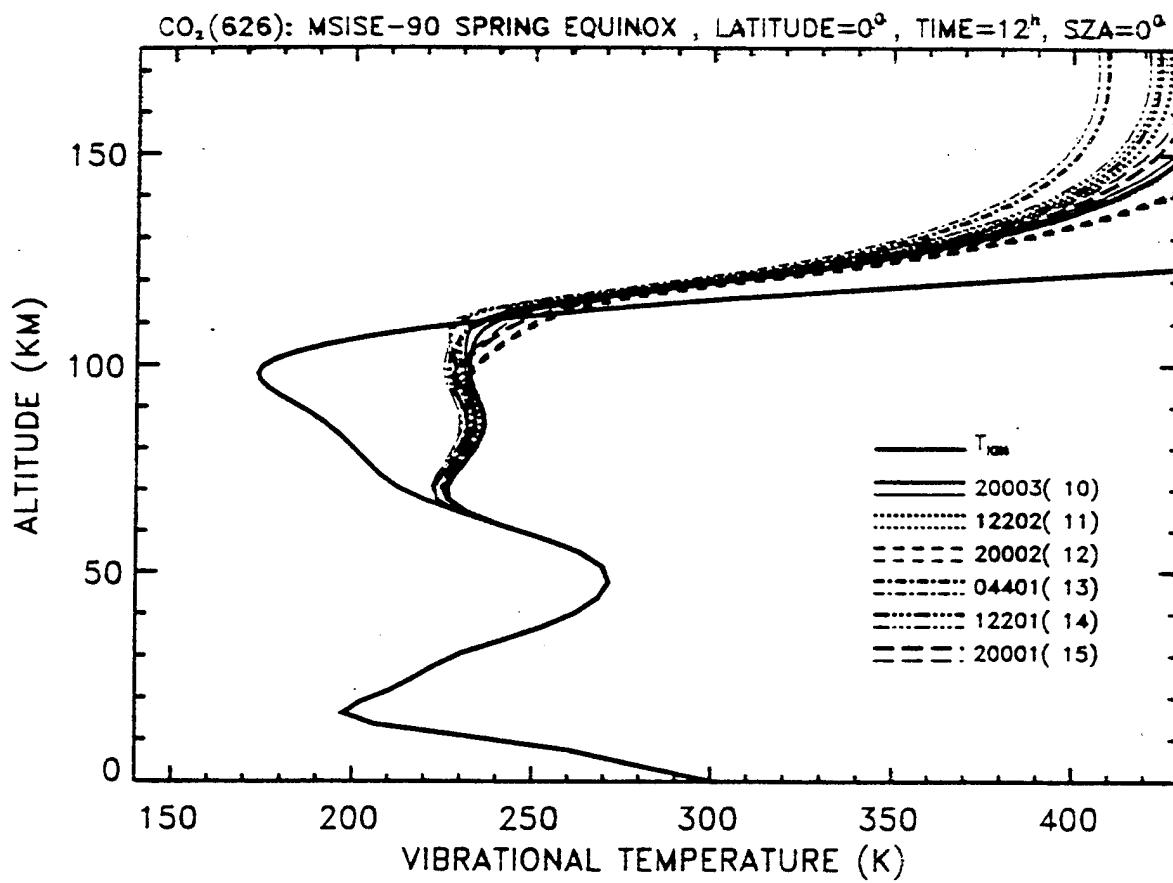




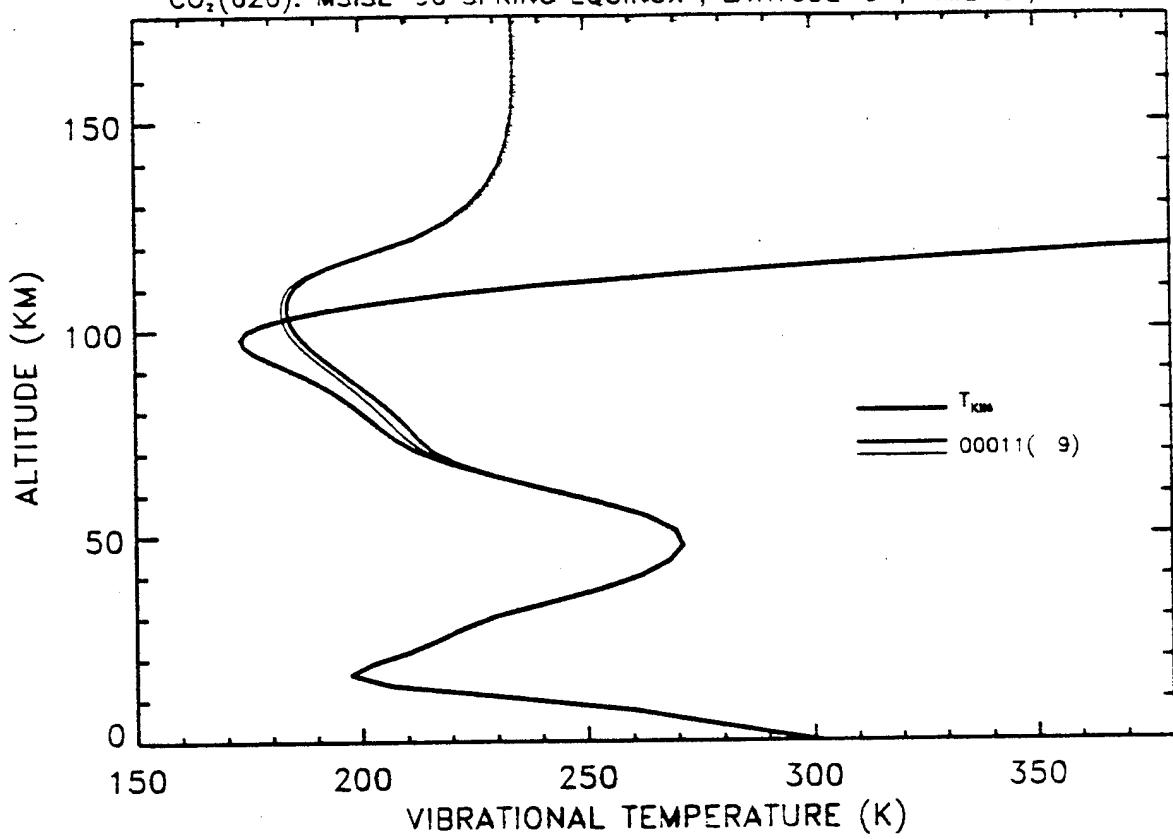


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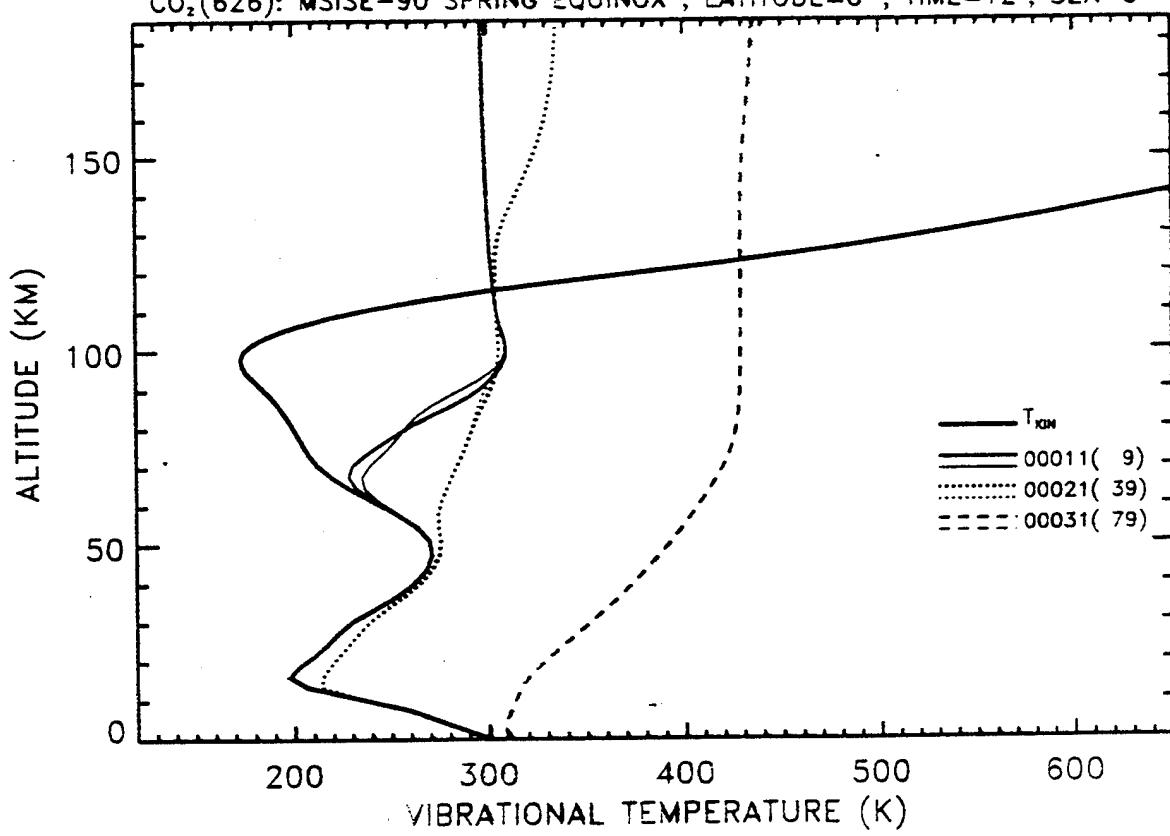


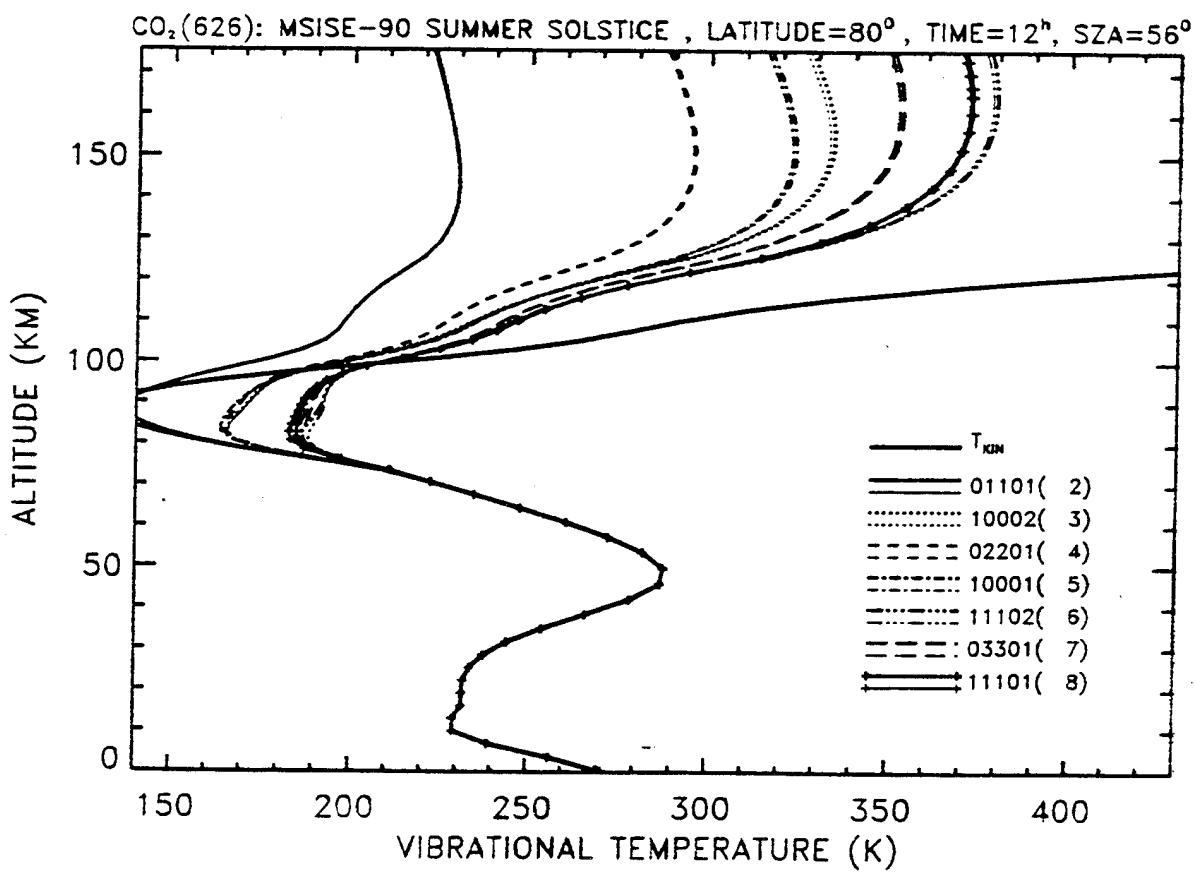
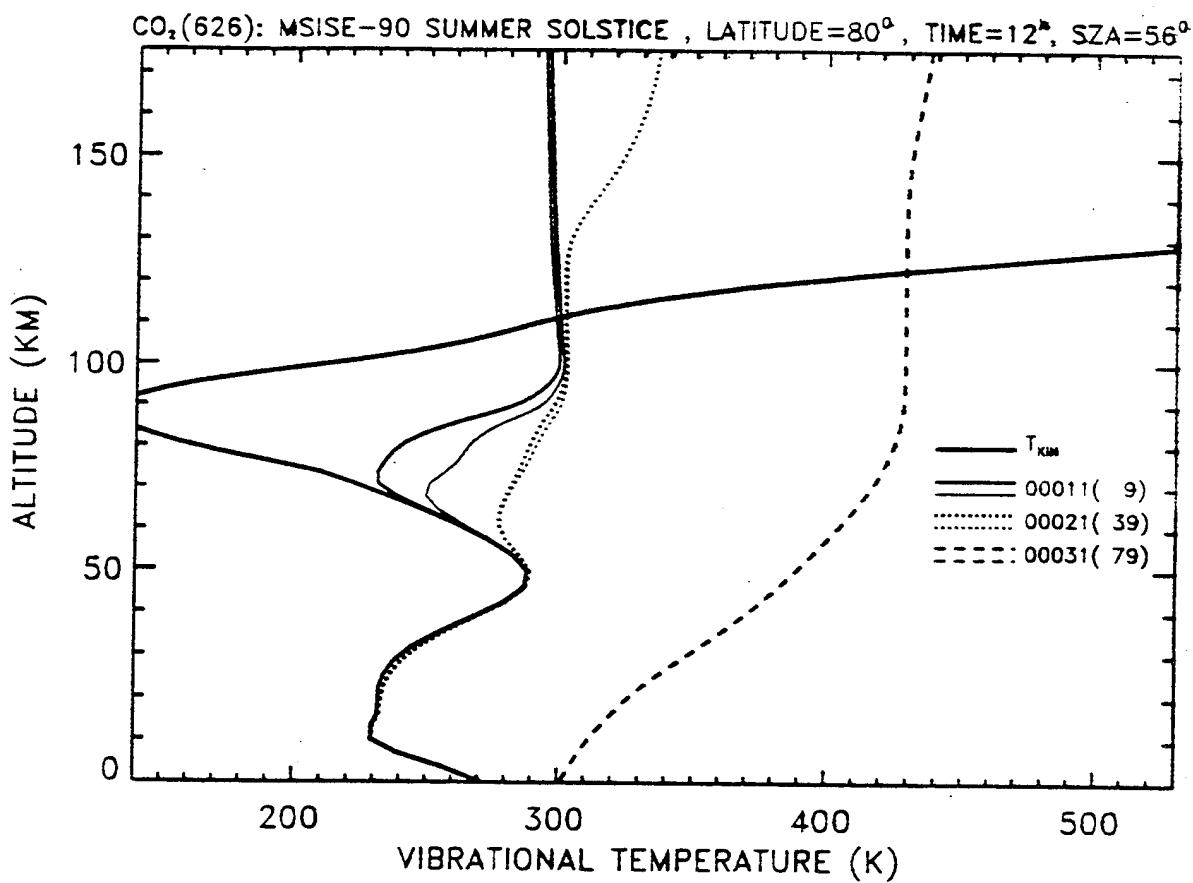


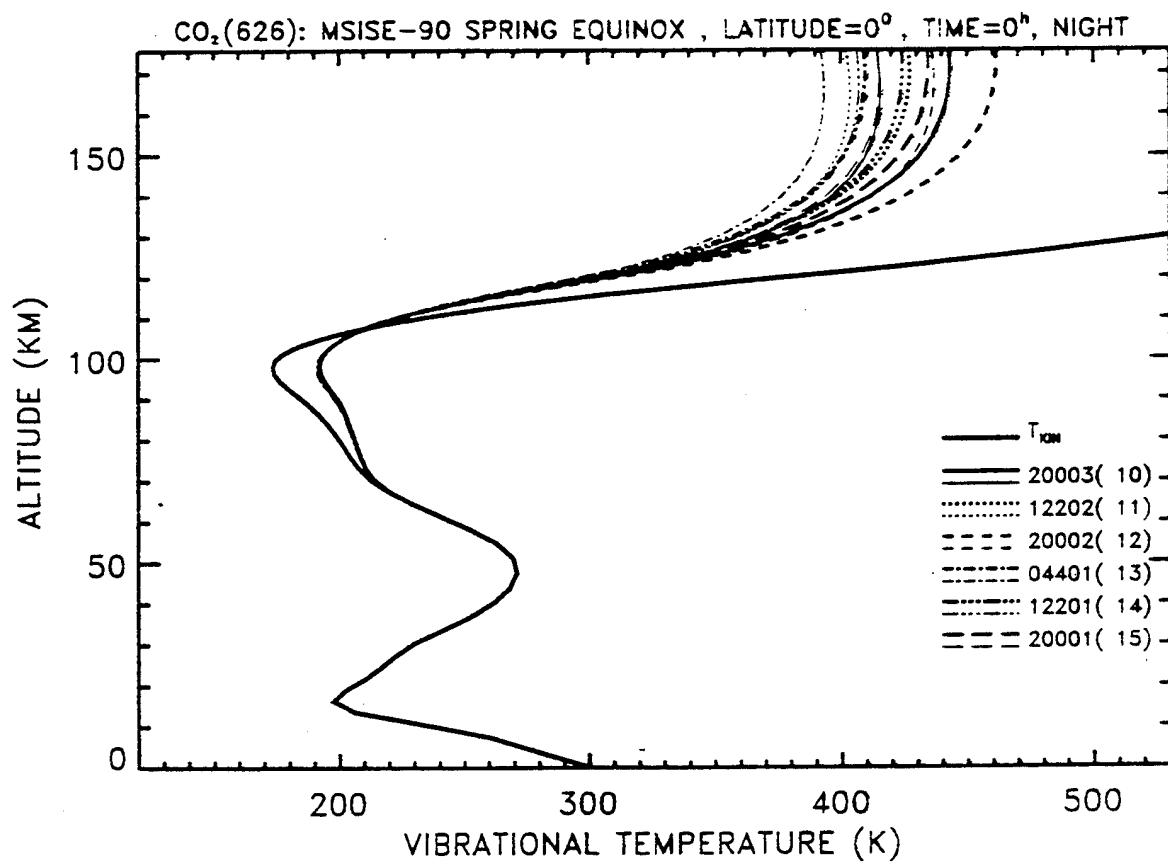
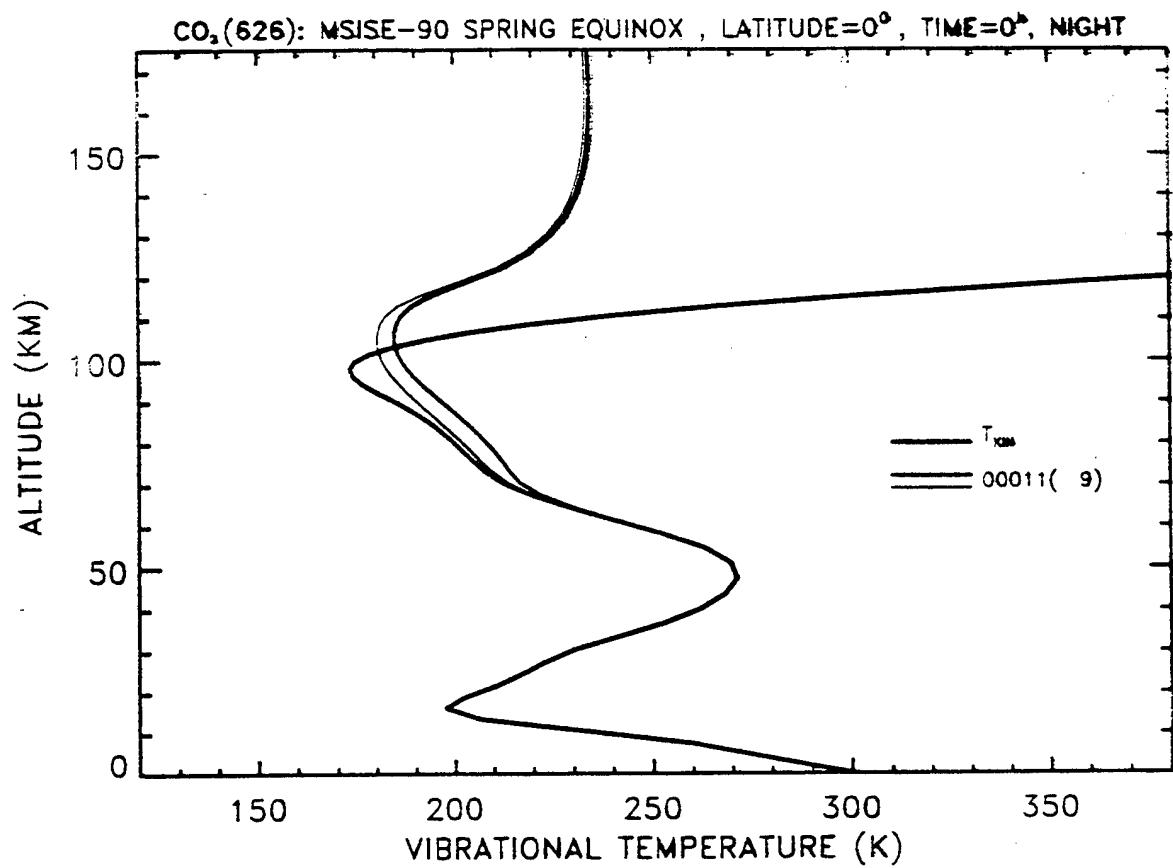
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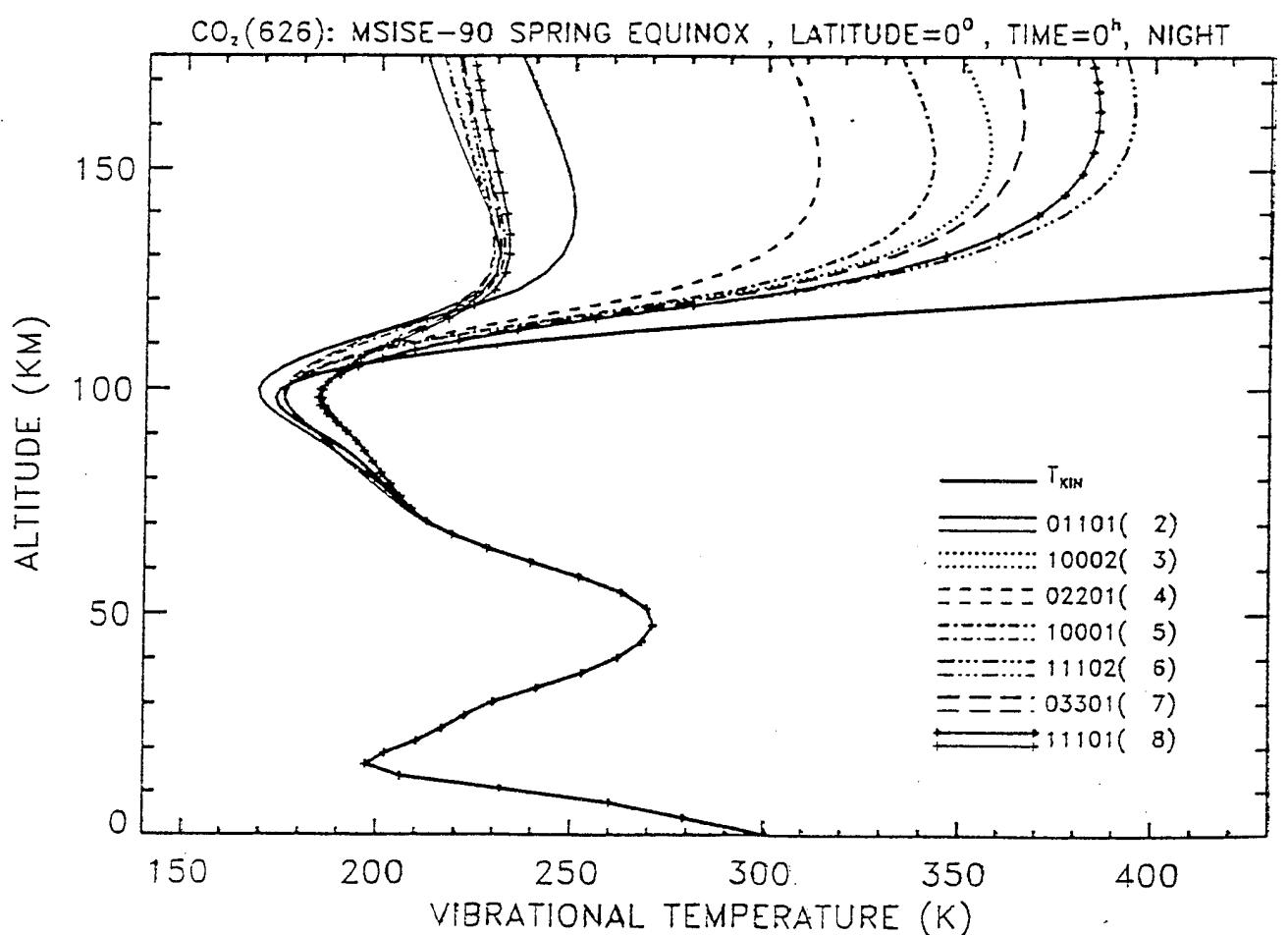
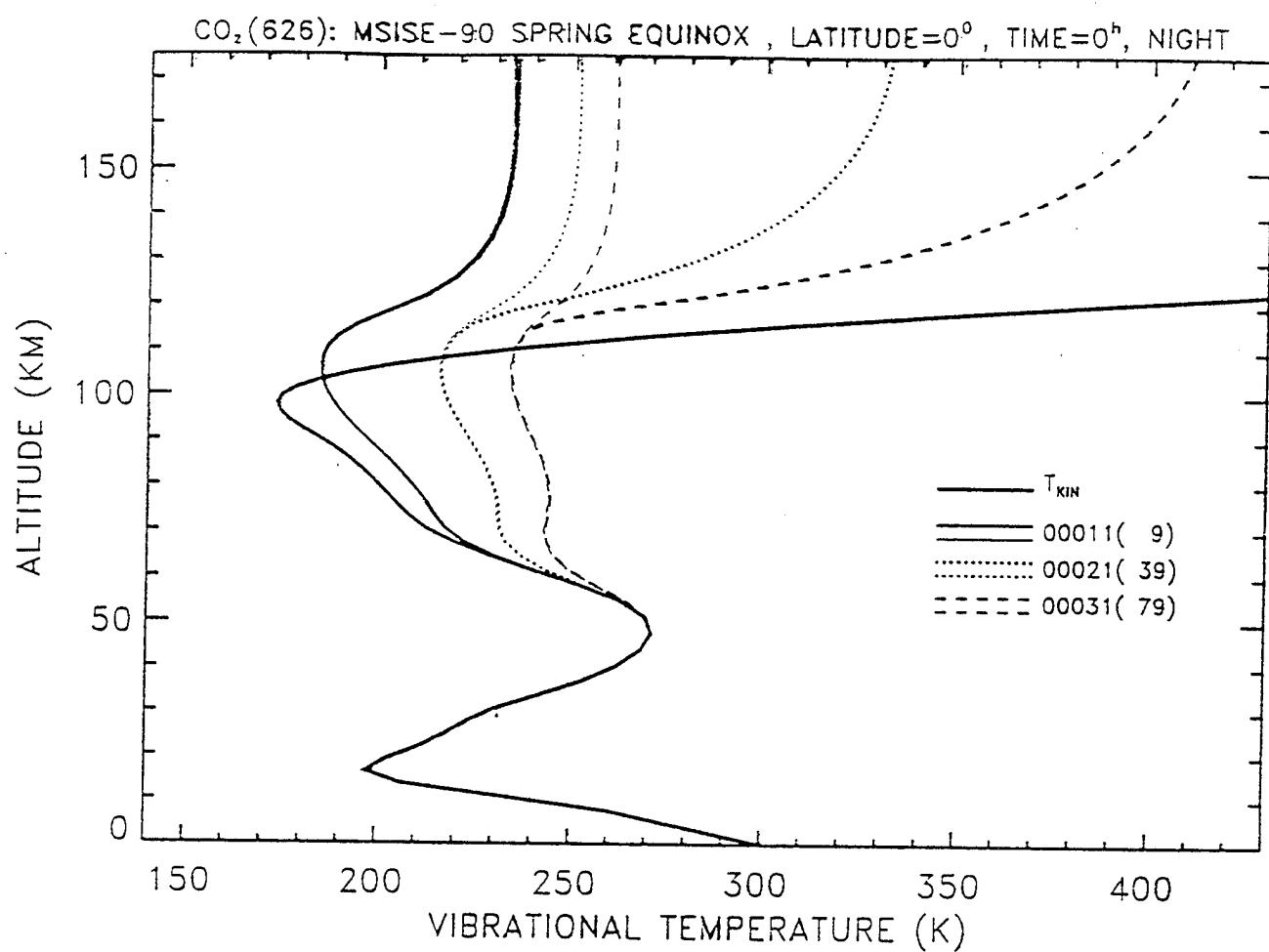


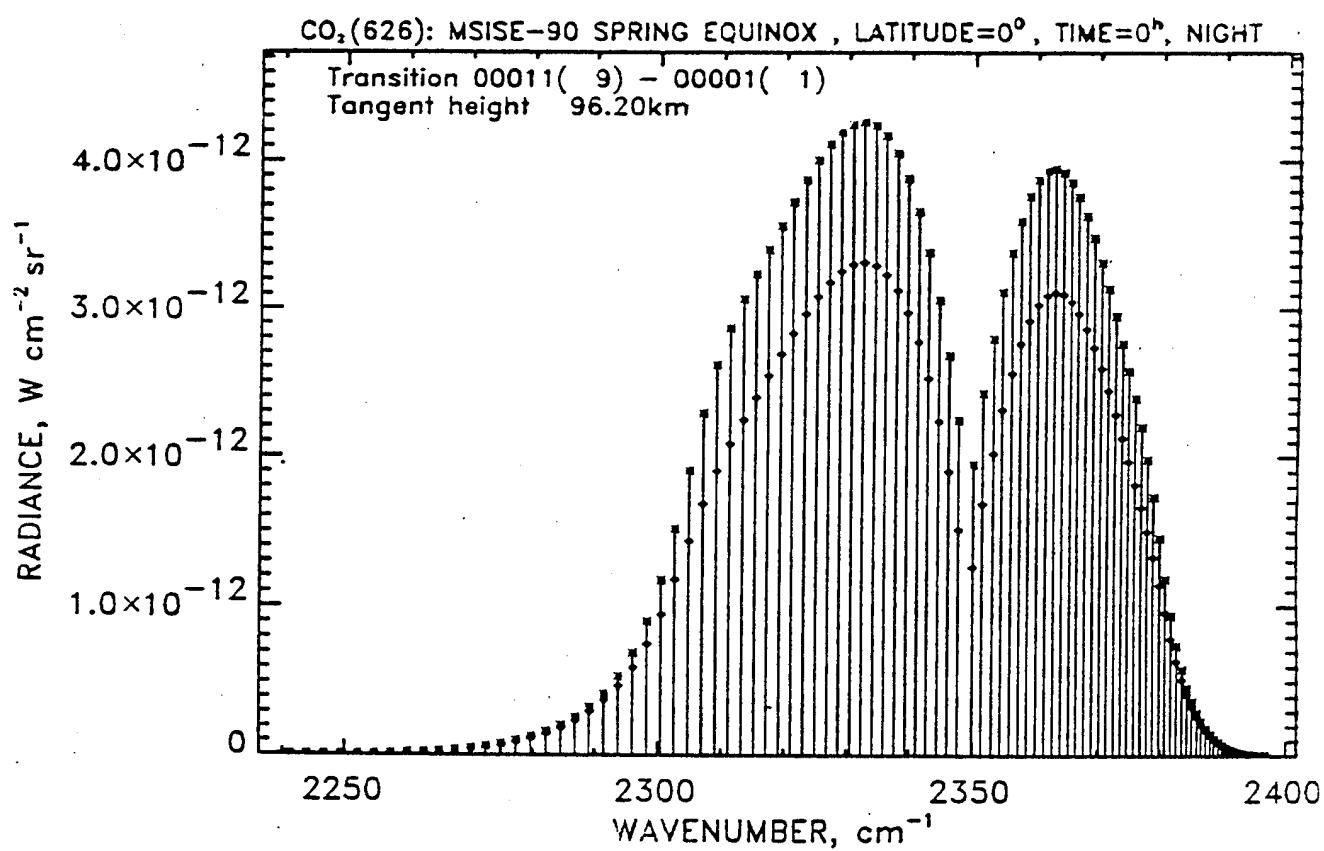
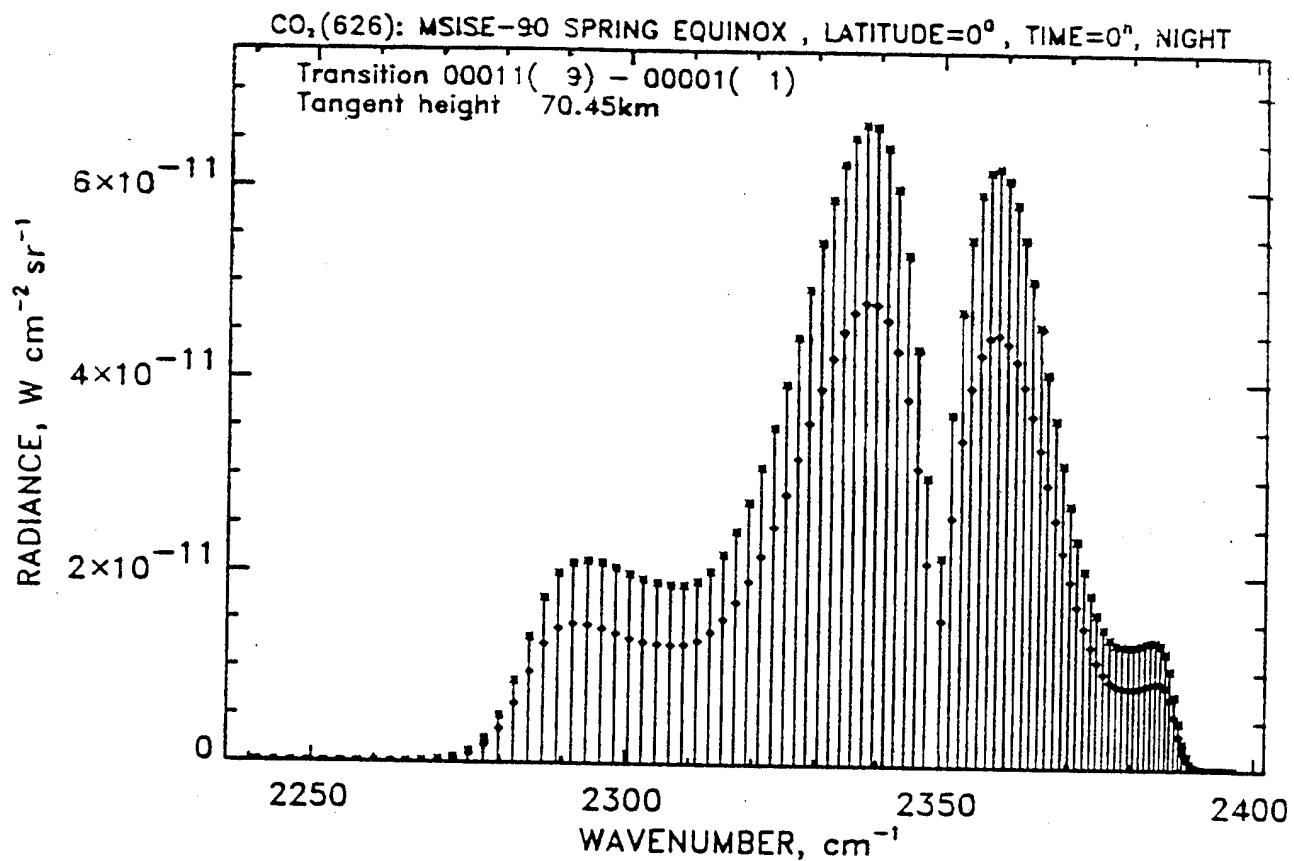
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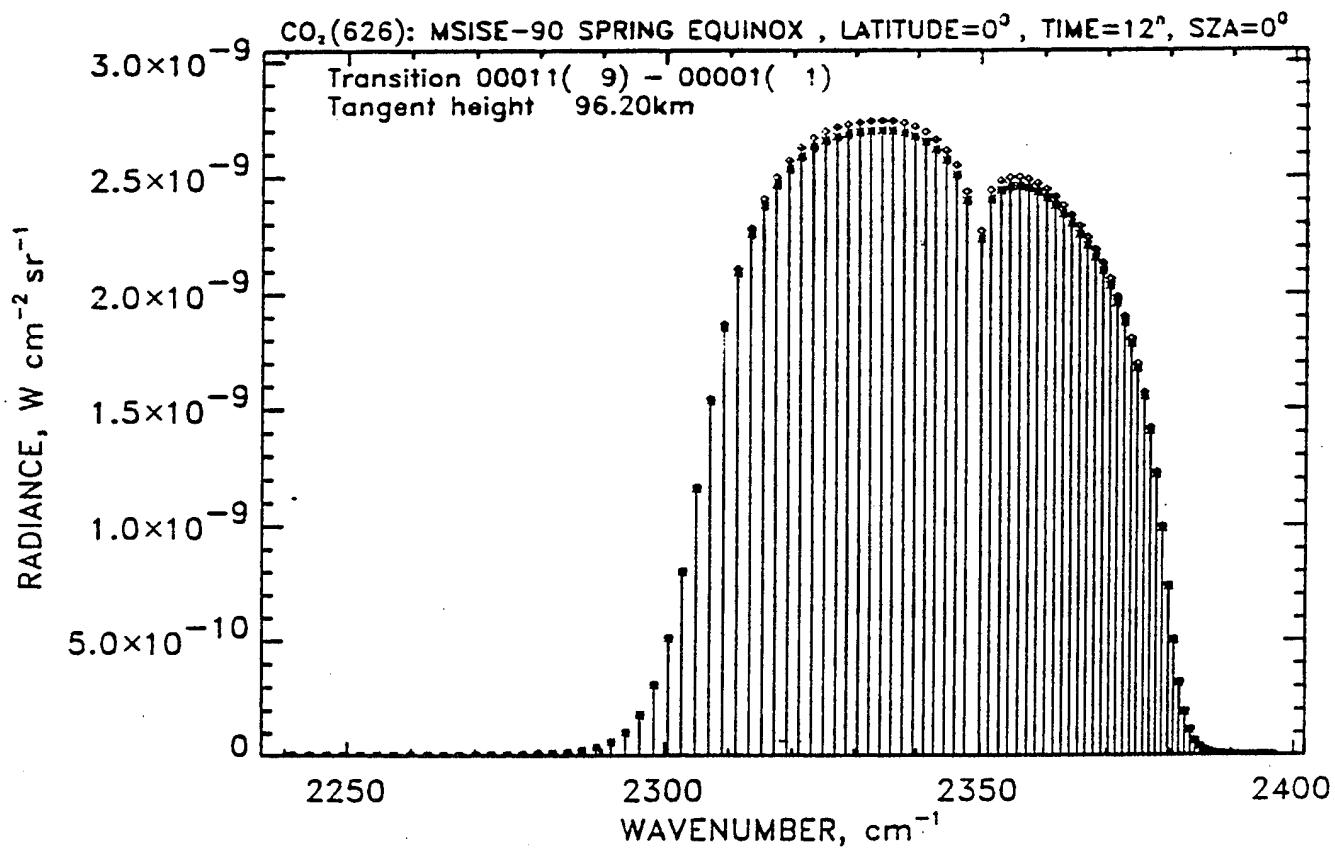
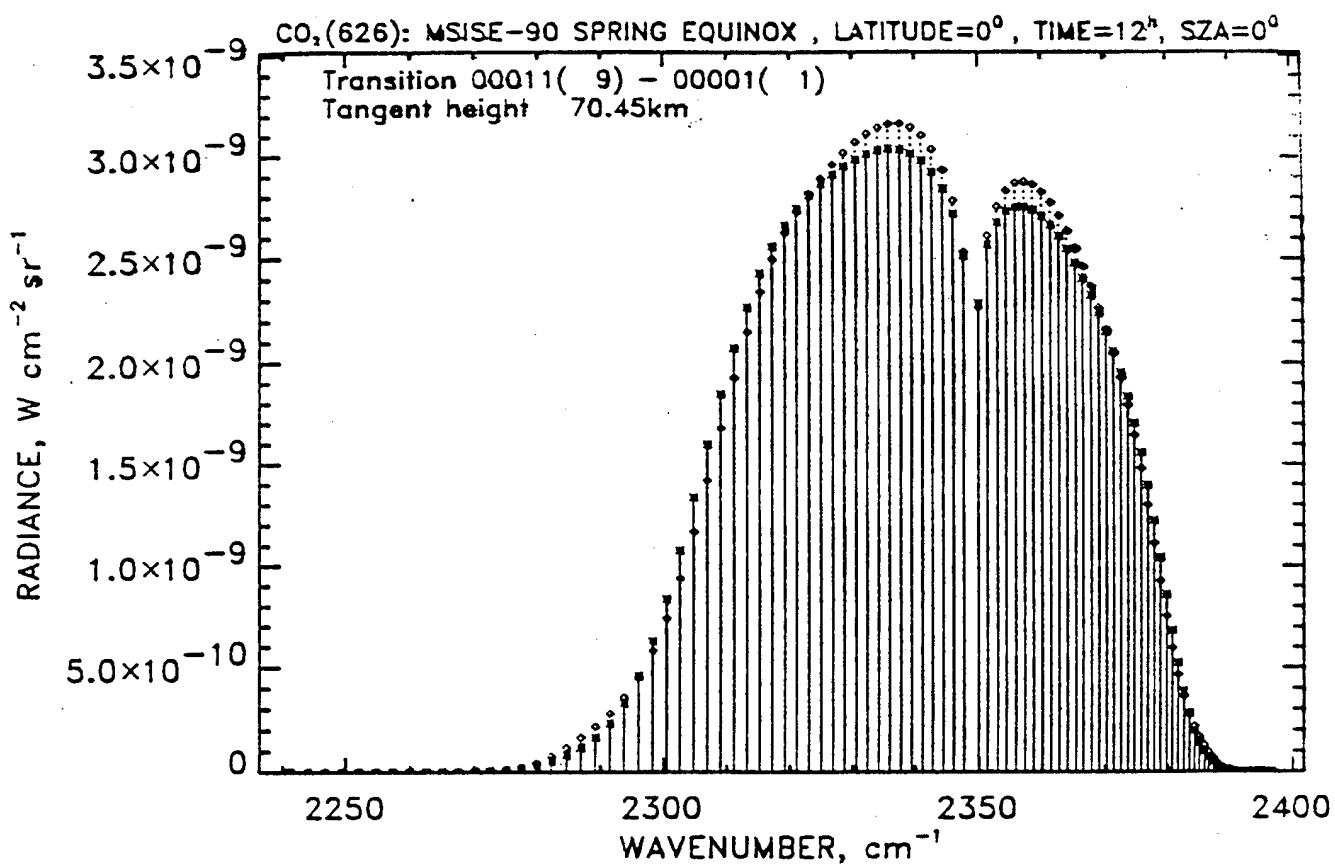


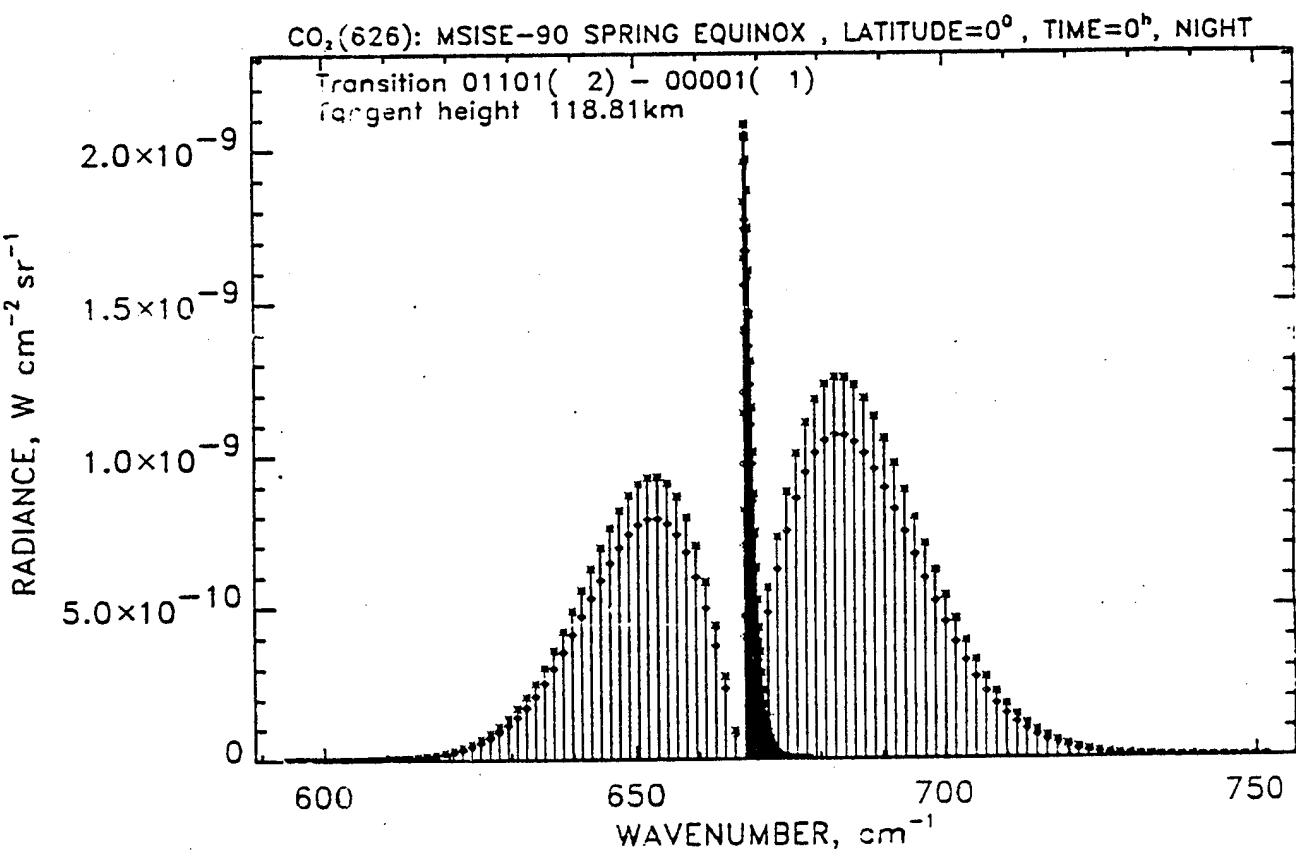
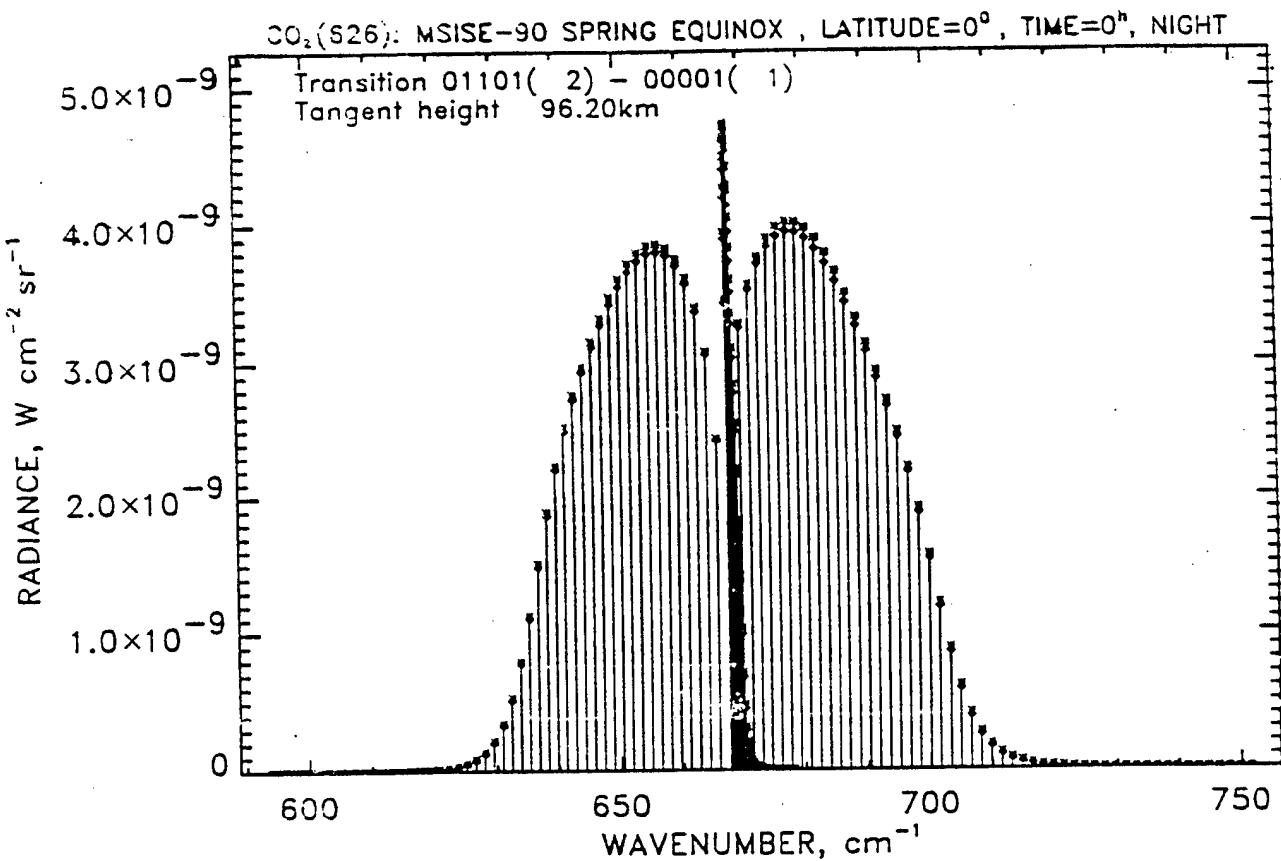


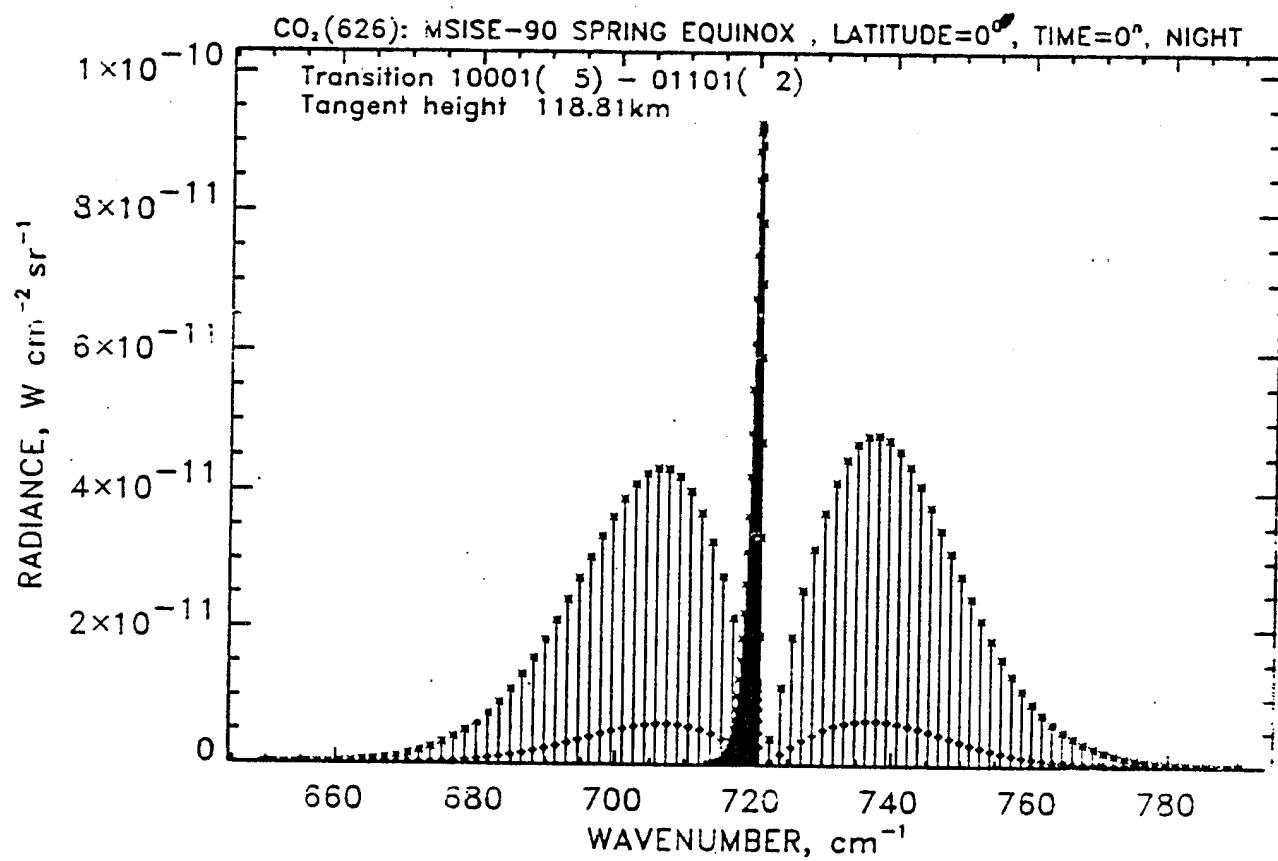
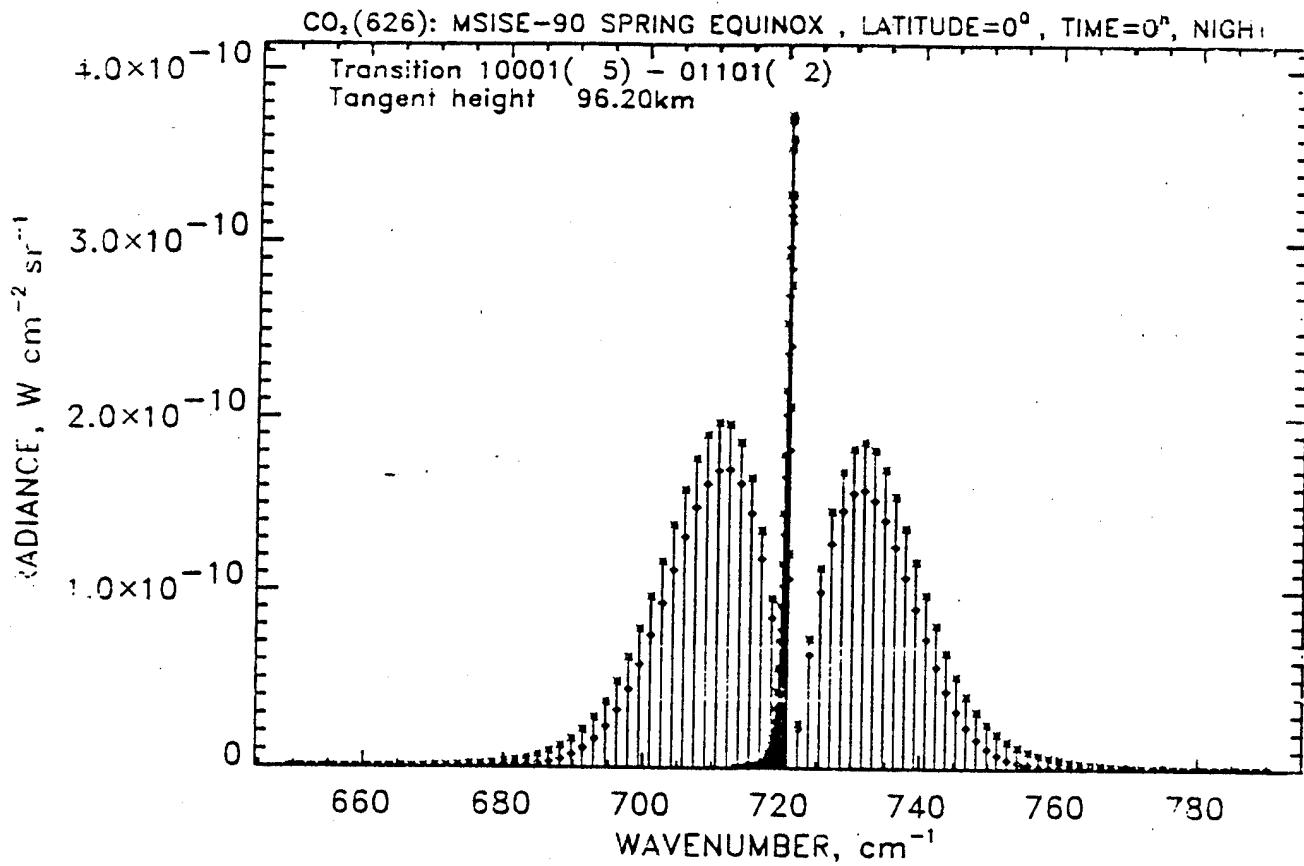


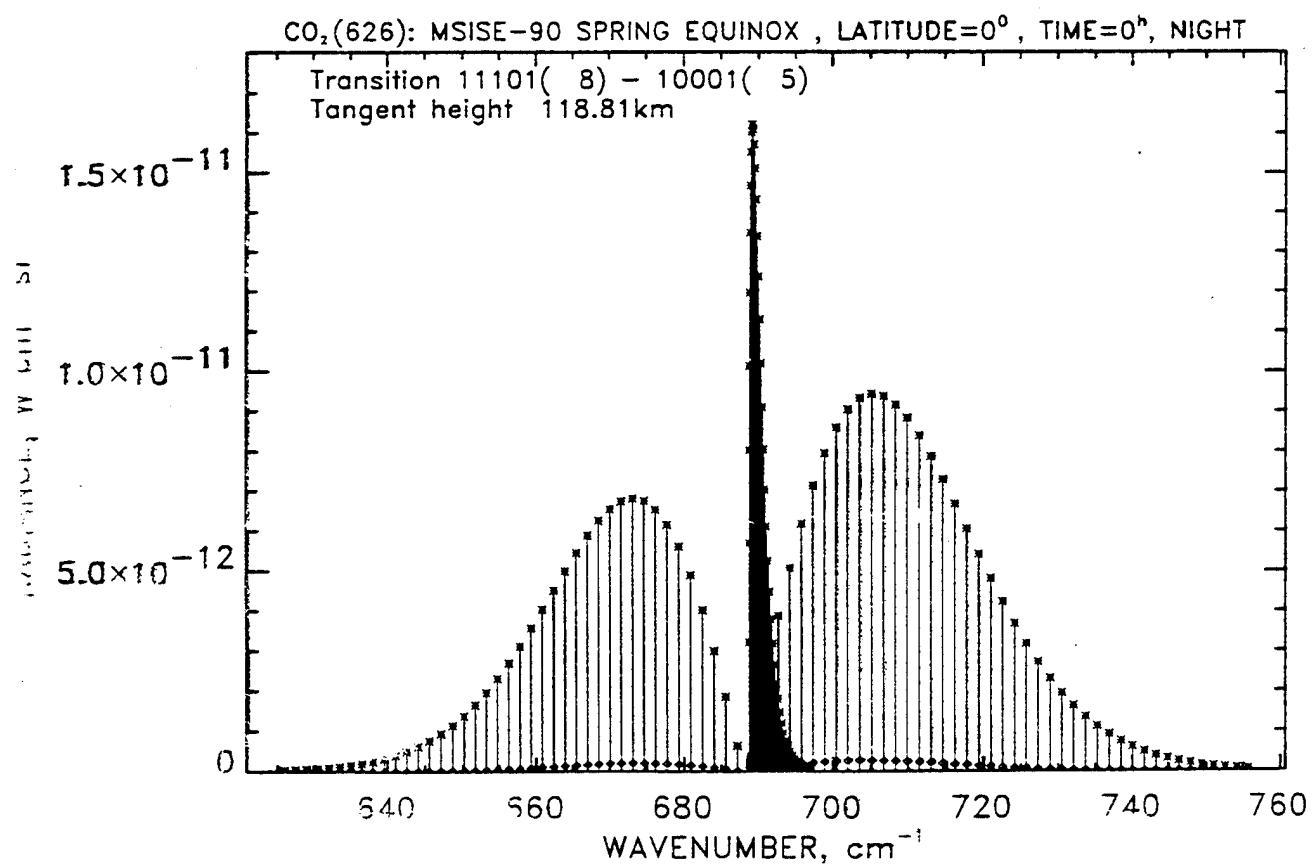
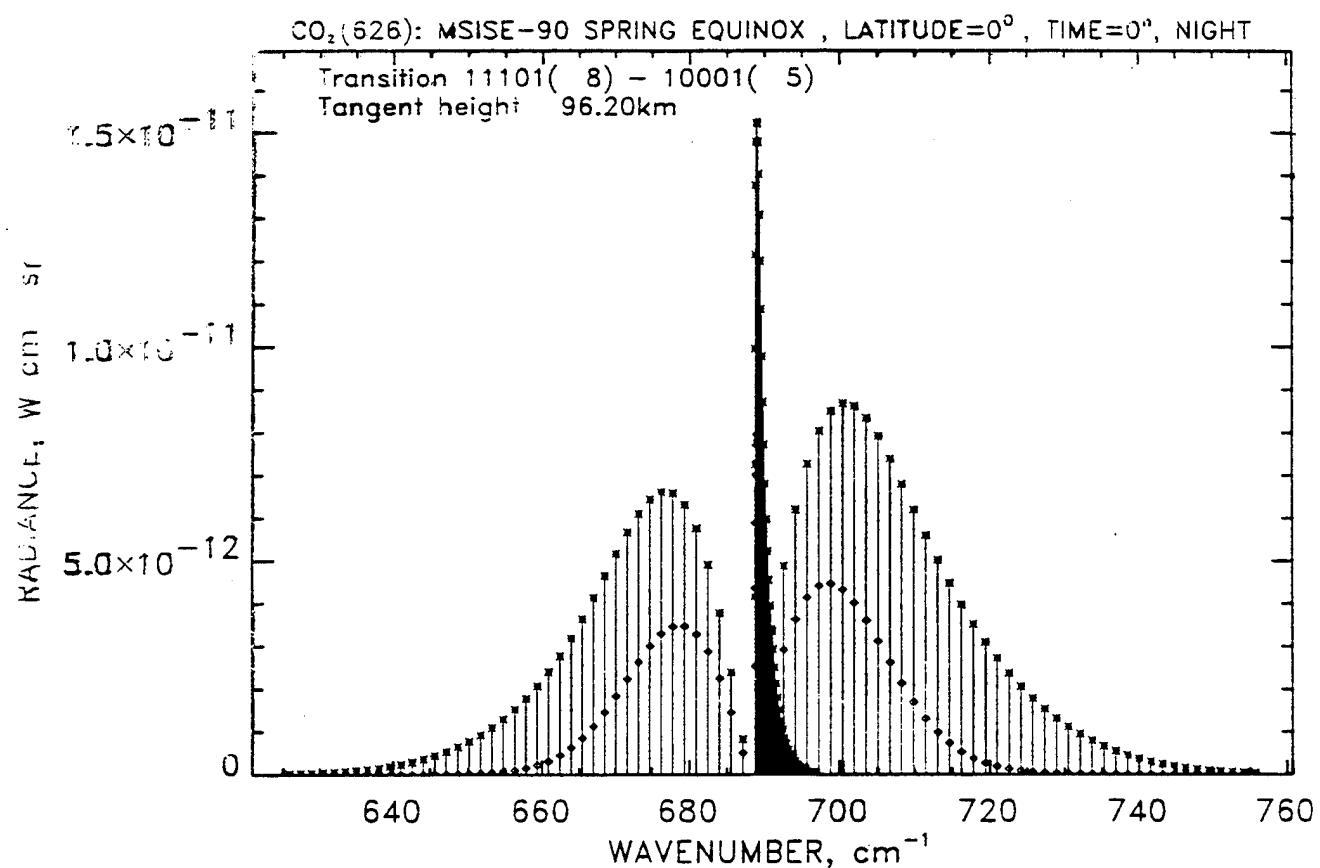


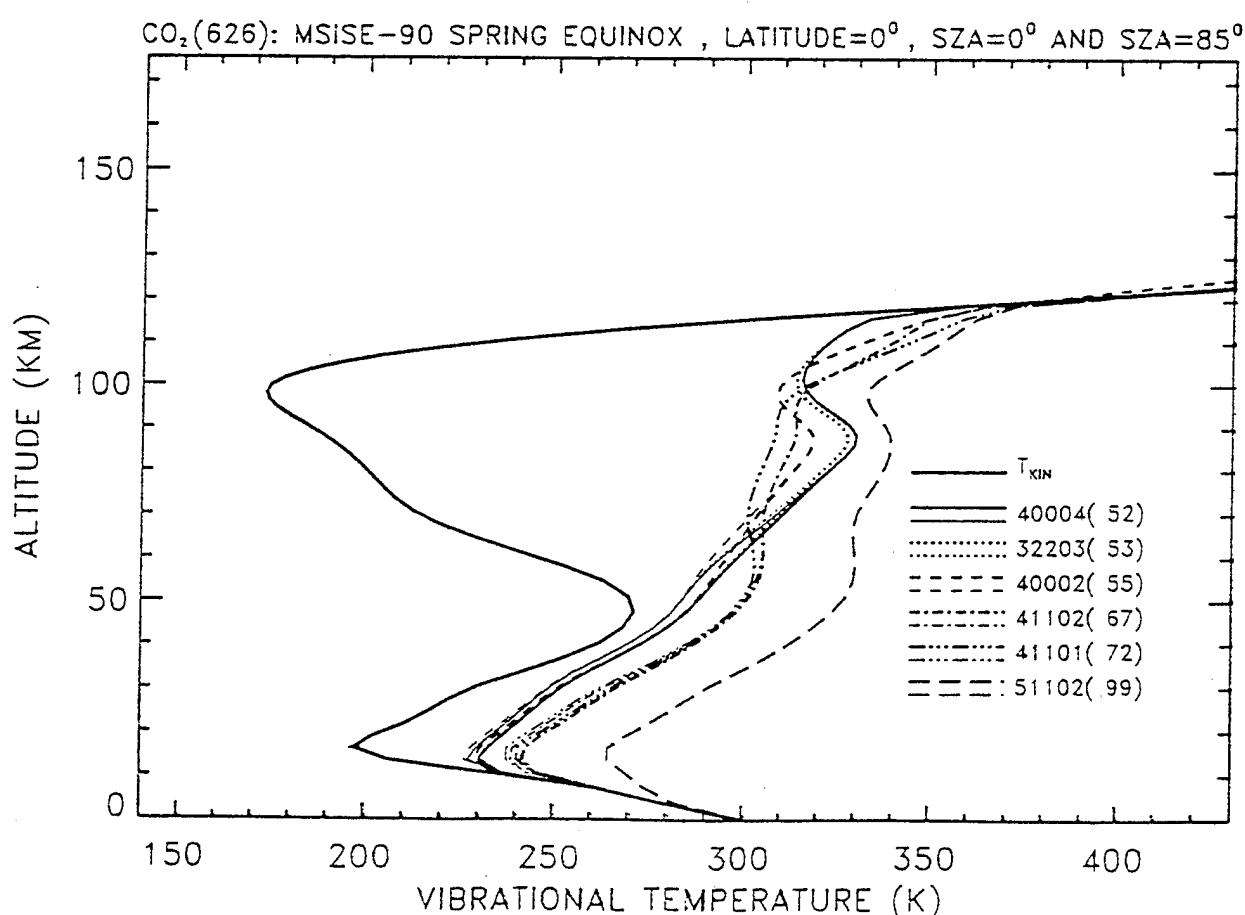
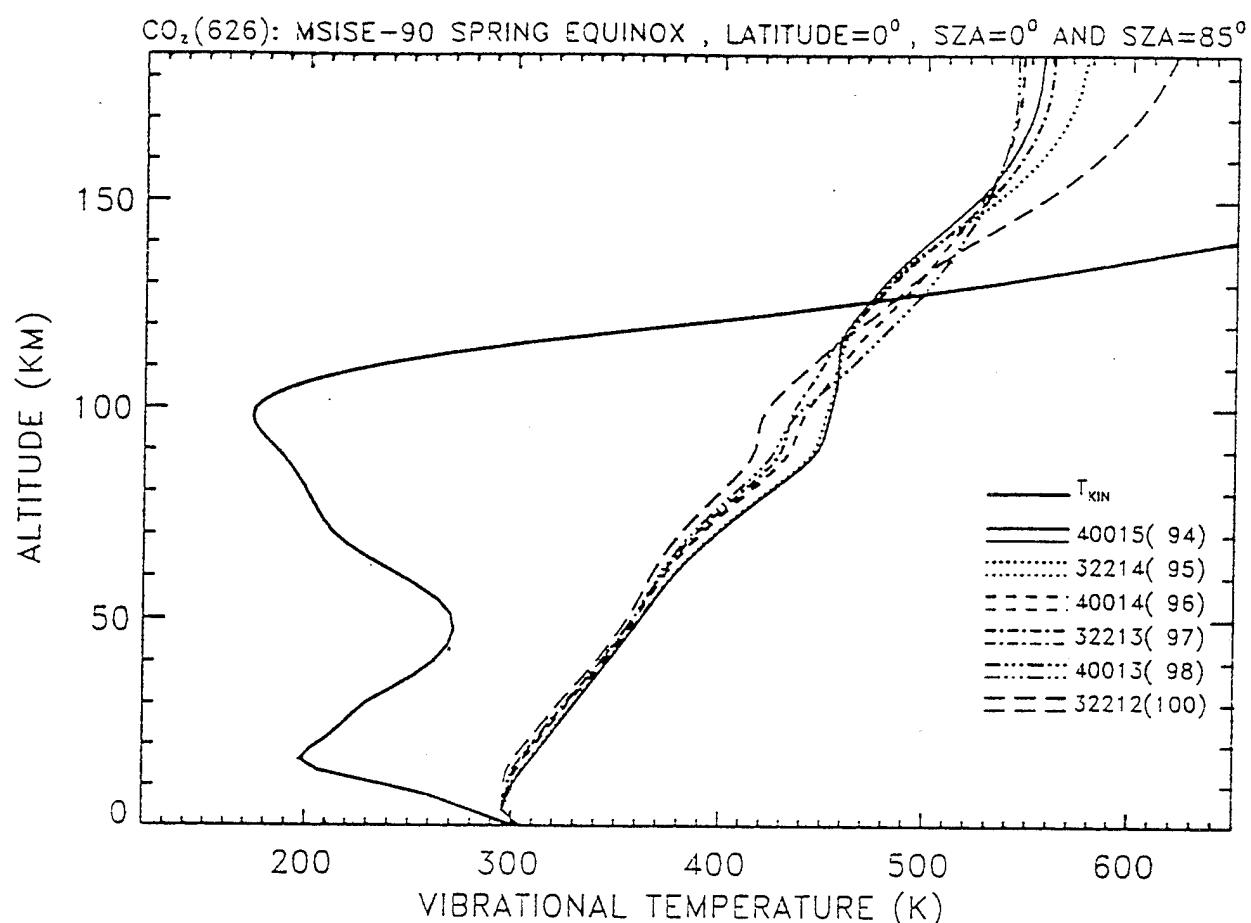












# Comparison of Line-by-Line and Modified Curtis Matrix Narrow-Band Model Approaches to Radiative Transfer in the CO<sub>2</sub> 15 micron Bands

P.P. Wintersteiner, ARCON Corporation, Waltham, MA  
M. Lopez-Puertas, Astrophysical Institute, Granada, Spain  
J.R. Winick, Phillips Laboratory, Geophysics Directorate  
R.H. Picard, Phillips Laboratory, Geophysics Directorate

17th Annual Review Conference  
on Atmospheric Radiation Models

June 8, 1994

## Objectives:

- Check validity of infrared radiative transfer methods by comparing band model with line-by-line approach
- Validate calculations of
  - CO<sub>2</sub> vibrational populations and emission rates
  - Atmospheric cooling by 15 micron emission
- Demonstrate capability of forward models for use with inversion/retrieval algorithms

## Approach:

- Isolate effects of the different radiative transfer methods by performing parallel calculations that are (otherwise) as nearly identical as possible
- Compare results:
  - Vibrational temperatures of CO<sub>2</sub> bend-stretch states
  - Atmospheric infrared cooling rates

# RAD Algorithm

- Iterative algorithm
  - Method of successive substitution
- Start with provisional vibrational temperatures
- Calculate radiative-excitation rates
- Recalculate vibrational temperatures assuming steady state
- Small equation set (different altitudes not explicitly coupled)
- Rapid convergence assured by nested iteration scheme
- Fundamental quantity: specific intensity of radiation
- Full line-by-line radiative transfer calculation
- Fully variable emission and absorption lineshapes
  - Dependence on temperature, pressure

# Modified Curtis Matrix (MCM) Model

- Inversion technique
  - Curtis Matrix method
  - Simultaneous solution of linear equations
  - Larger equation set (different altitudes explicitly coupled)
- Fundamental quantity: heating rate
- “Pseudo” line-by-line algorithm
  - Numerical integration over frequency
  - Reduced number of equivalent lines, grouped by strength
- Averaging over atmospheric paths
  - Curtis-Godson approximation
  - Lineshape, temperature, density, pressure

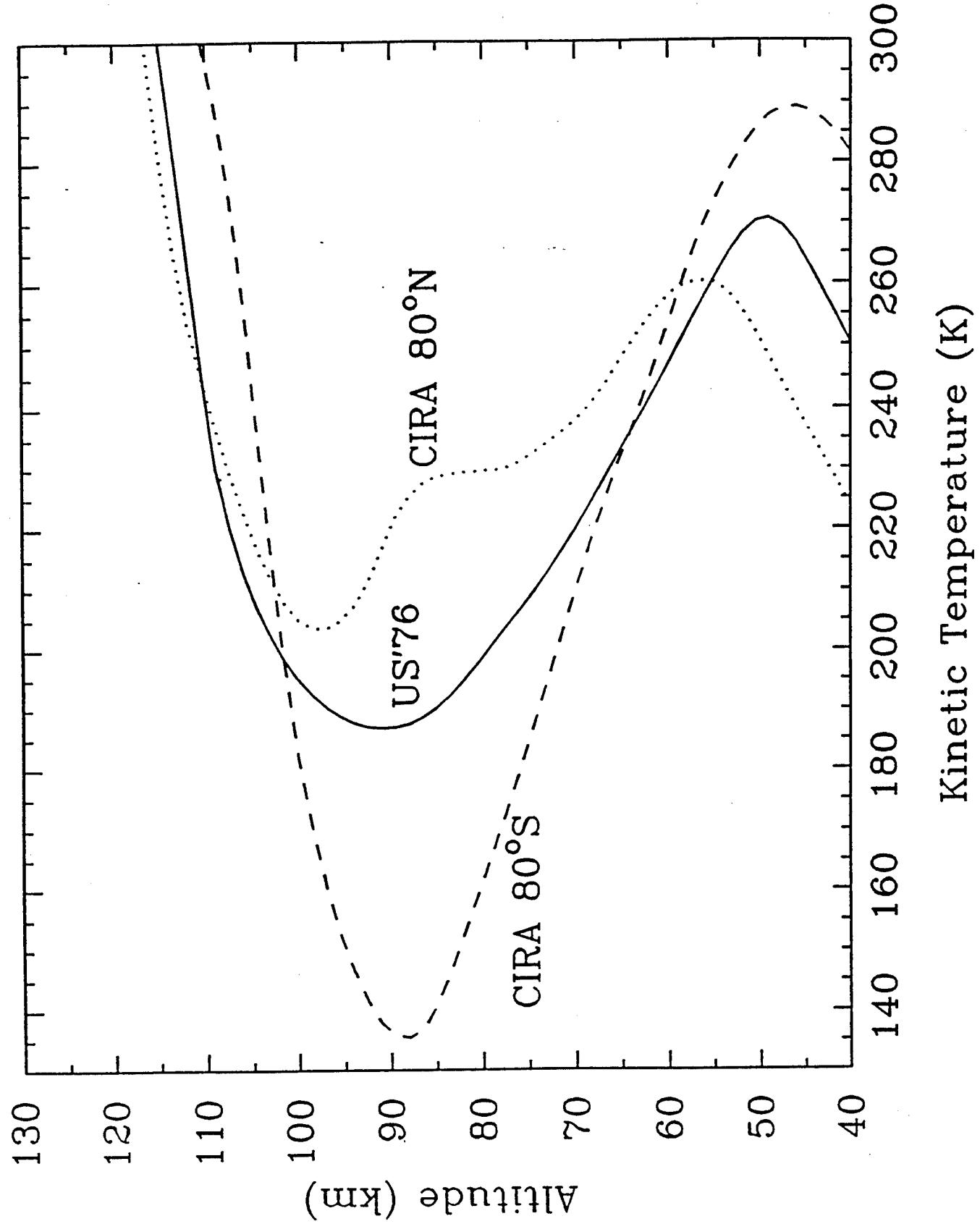
# Correlating the Models

- Input model atmospheres
  - Temperature, constituent densities
  - Layering: 80 layers, 40-160 km, 1.5 km/layer
- Thermal and vibrational mechanisms
- Rate constants for collisional processes
- Radiative transition data
  - 626 fundamental, minor isotope fundamentals, 626 hot bands
  - HITRAN'92 lines
  - Temperature dependence of line strengths
- CO<sub>2</sub> isotopic abundances
- Treatment of lower boundary

# Test Cases

- Model Atmospheres
  - US Standard Atmosphere, 1976 (midlatitude, “average” structure)
  - CIRA 80 degrees S, December (warm stratopause, cold mesopause)
  - CIRA 80 degrees N, December (cold stratopause, warm mesopause)
- Rate constant for deactivation of bending mode by [O]
  - “Fast” case:  $k_o = 6.1 \times 10^{-12} \text{ cm}^3 / \text{sec}$  @ 300 K  
(Sharma and Wintersteiner, GRL 17, 2201, 1990)
  - “Slow” case:  $k_o = 2.0 \times 10^{-13} \text{ cm}^3 / \text{sec}$  @ 300 K

## Model Atmospheres



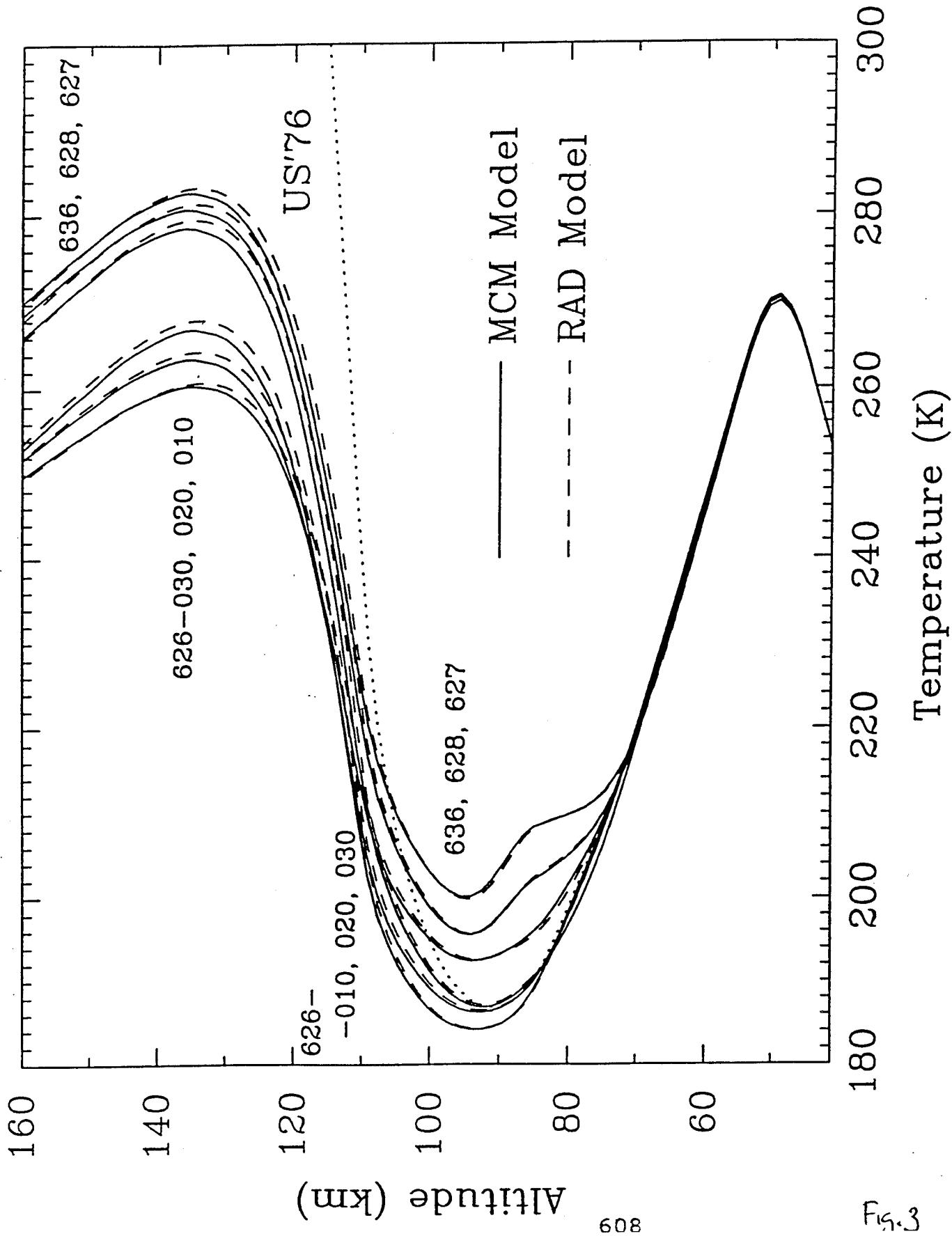
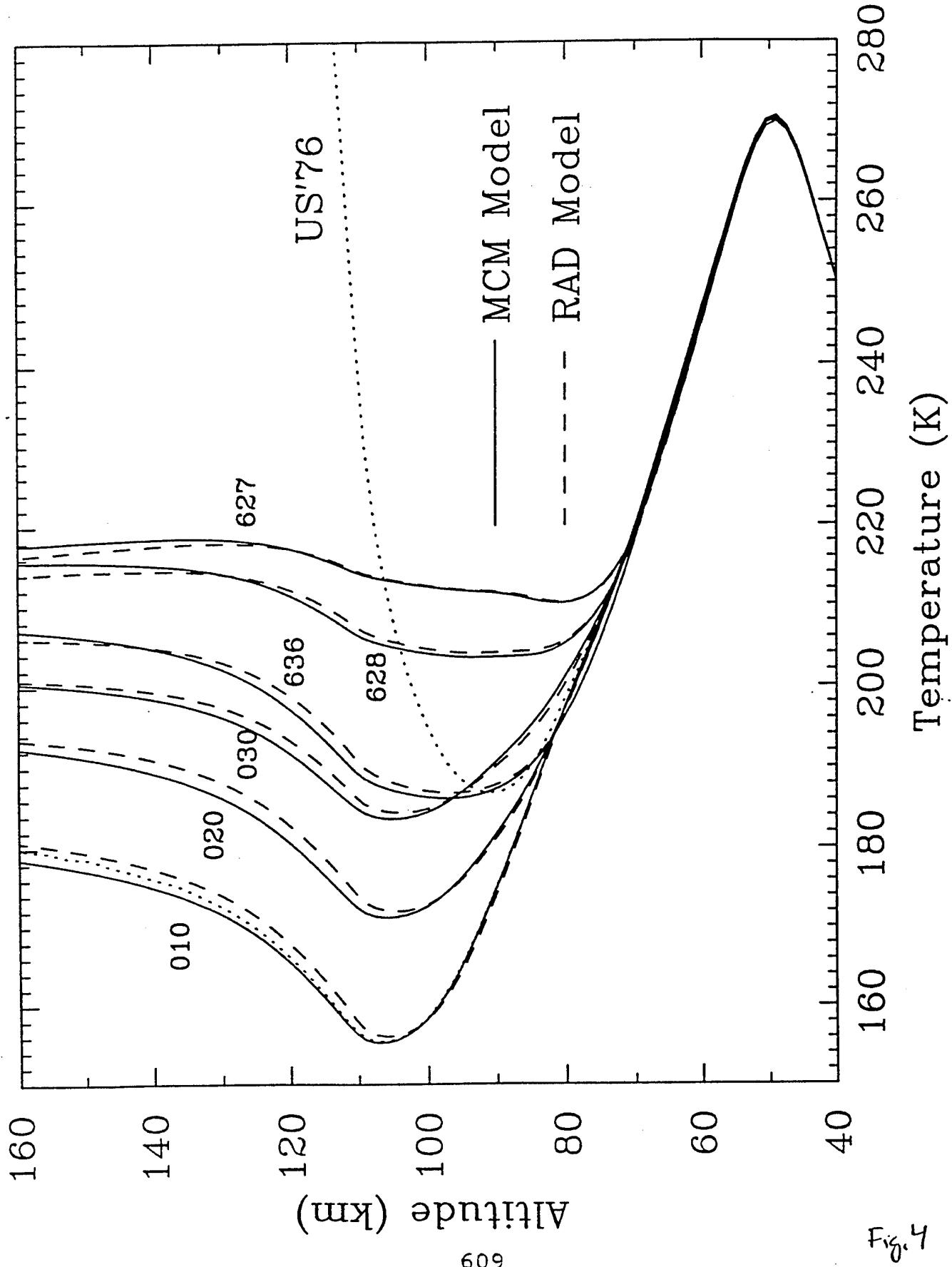


Fig. 3



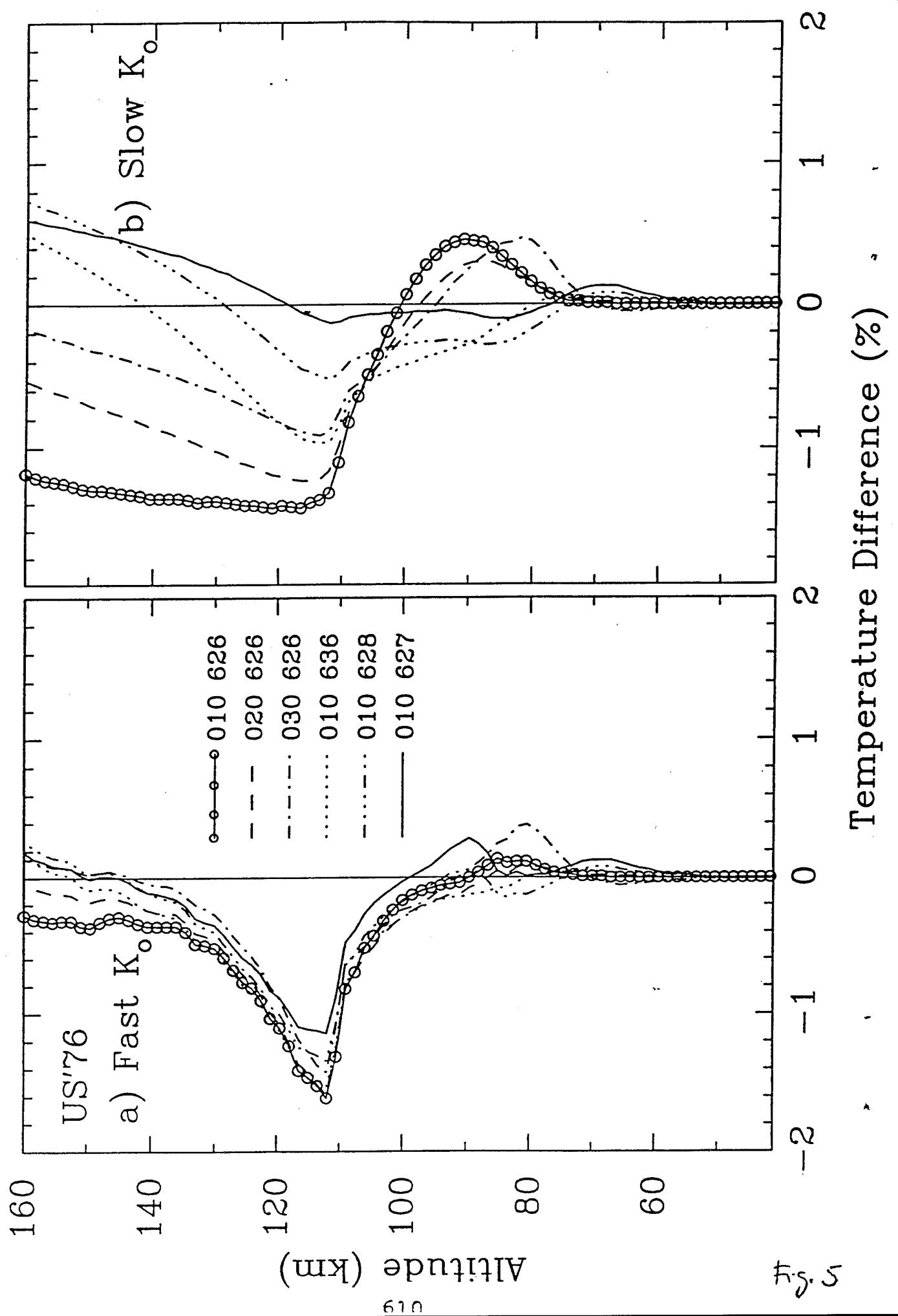


Fig. 5

# Summary of Results, Vibrational Temperatures

- “Fast” case (realistic kinetic parameters)
  - Below 70 km, excellent agreement
  - In the upper mesosphere
    - absolute differences < 1 K, for US'76 and CIRA 80 N, all bands
    - absolute differences < 2 K for CIRA 80 S except 626-030 (< 3 K)
    - 626-010 level quite close to LTE at summer polar mesopause
  - In the thermosphere
    - MCM consistently predicts lower vibrational temperatures
    - peak differences < 4 K, occurring near 115-120 km
- “Slow” case (best test of radiative transfer)
  - Absolute differences < 2.5 K for US'76 and CIRA 80 N, all bands
  - Differences < 3 K (mesosphere) or 6 K (thermosphere) for CIRA 80 S
  - MCM consistently predicts
    - lower vibrational temperatures in the thermosphere
    - higher vibrational temperatures at the mesopause

# Understanding Models' Differences

- Issue
  - MCM underestimates total radiative excitation in thermosphere
  - MCM overestimates total radiative excitation near mesopause
- Take MCM to “line-by-line limit”
  - Eliminate grouping of equivalent lines
  - Better agreement in thermosphere
  - General pattern of discrepancies persists
- Analyze total radiative excitation in thermosphere
  - Compare contributions from different source layers
  - MCM calculates
    - less absorption from source layers below the mesopause
    - more absorption from source layers above the mesopause

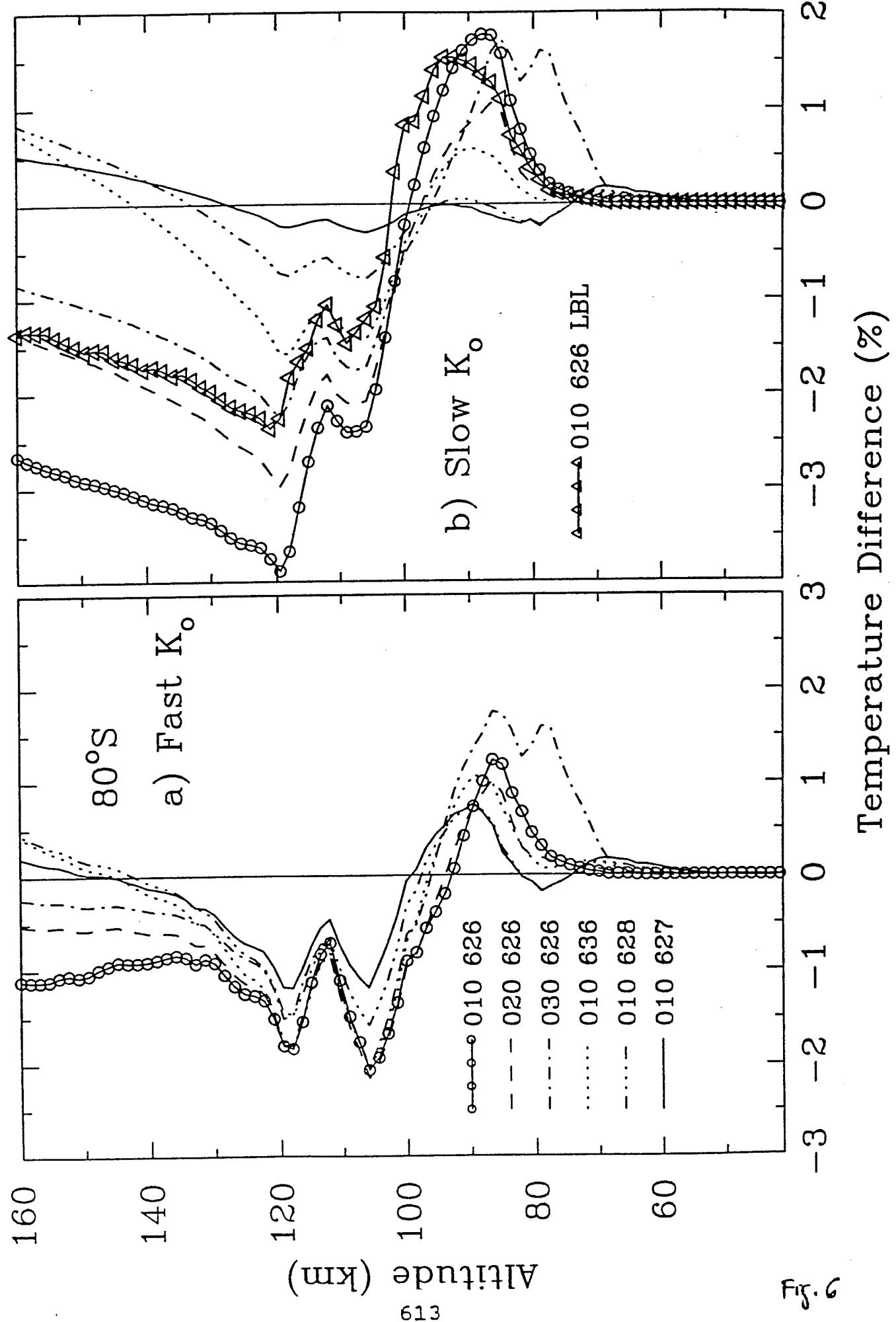
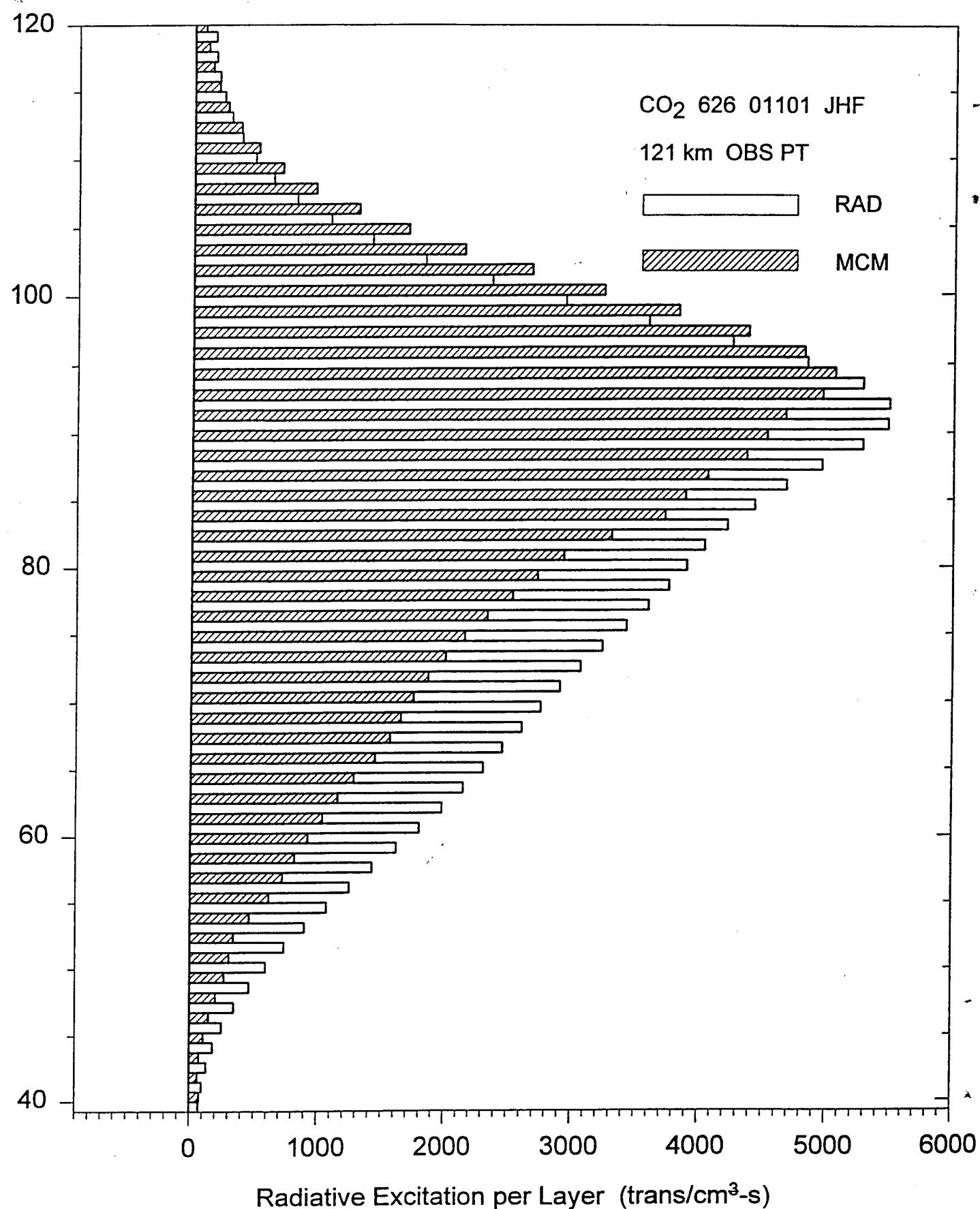


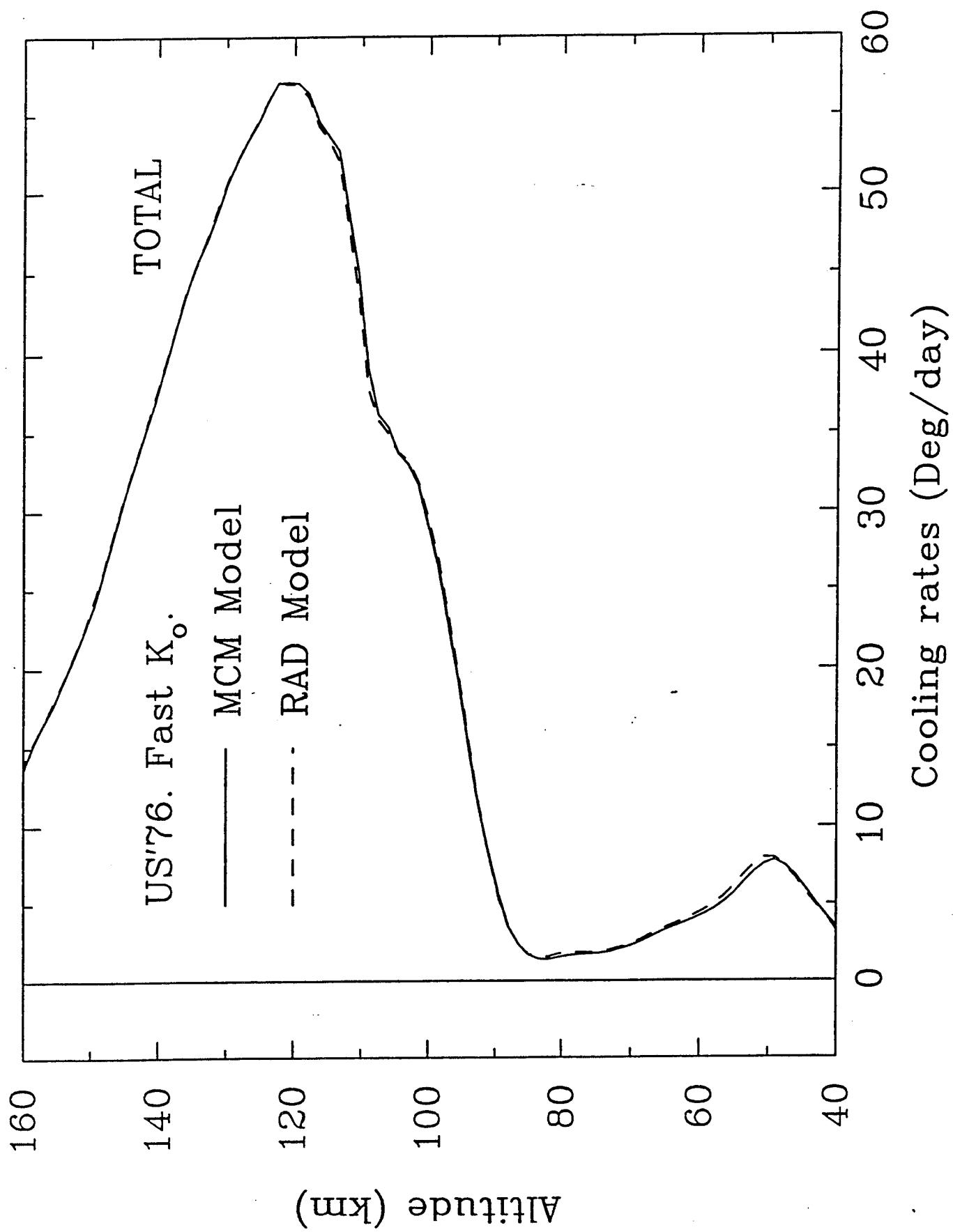
Fig. 6

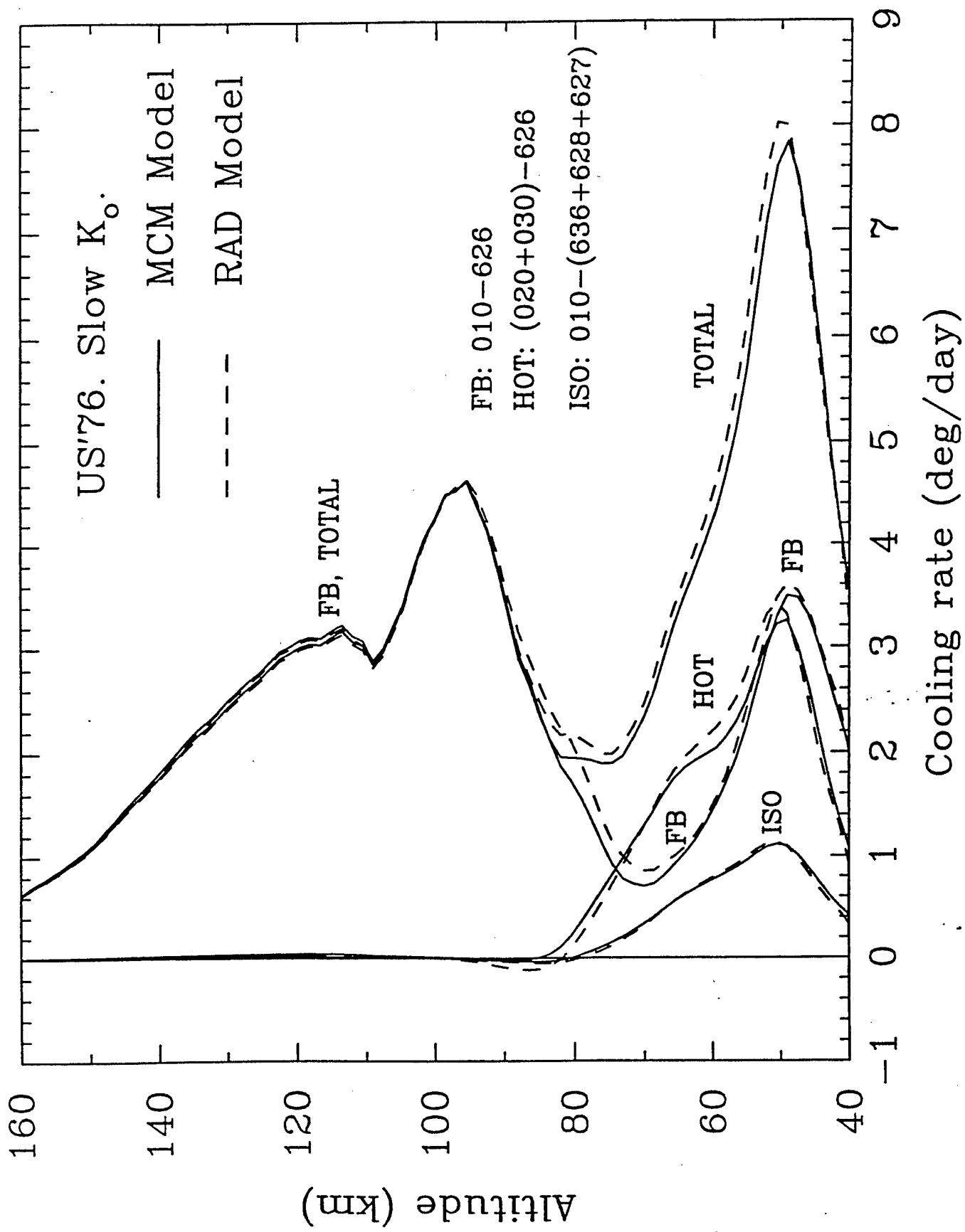
## Total Radiative Excitation



# Understanding Models' Differences (cont.)

- MCM path-weighted temperature smaller than proper absorption temperature; path-weighted pressure greater absorption lineshape narrower than in RAD
  - less absorption in wings (lower-altitude, warmer source regions)
  - more absorption in line centers (higher-altitude, colder source regions)
- Result: MCM calculates less total radiative excitation in thermosphere
  - Analyze radiative excitation at the mesopause
- MCM path-weighted temperature greater than proper absorption temperature; path-weighted pressure greater absorption lineshape broader than in RAD
  - more absorption in wings (lower-altitude, warmer source regions)
  - less absorption in line centers (higher-altitude, colder source regions)
- Result: MCM calculates more total radiative excitation at mesopause
  - Residual discrepancies explained by MCM path-averages





# Summary of Results, Cooling

- Lower mesosphere
  - Absolute differences  $< 0.5 \text{ K/day}$  ( $\sim 6\text{-}8\%$  of total cooling)
  - Agreement consistent for all bands
- 626 fundamental  
isotopic fundamentals  
hot bands
- “Fast” and “slow” cases give the same results
- Mesopause and thermosphere
  - Differences significant only for “fast” case
  - Absolute differences  $< 3 \text{ K/day}$ , all altitudes
  - Peak differences occur in narrow altitude ranges

## Conclusions

- The two radiative transfer algorithms give consistent results for populations and cooling
  - Strong and weak bands
  - 120-km altitude range
  - Extreme temperature structures
  - Extreme kinetic parameters
- Small discrepancies understood
  - Grouping of equivalent lines in MCM
  - Path-average temperature, pressure, affect absorption lineshape in MCM
- Vibrational temperatures and cooling rates validated
  - Results are accurate enough to be used for retrievals from non-LTE atmospheric emissions
  - Cooling rates are accurate enough for use in dynamical models and thermal-balance calculations



# Subthermal NO( $^2\Pi_{\Omega}$ ) Spin-Orbit Distributions in the Thermosphere

S.J. Lipson, P.S. Armstrong<sup>1</sup>, J.A. Dodd<sup>1</sup>,  
J.R. Lowell, W.A.M. Blumberg, and R.M. Nadile  
Phillips Laboratory, Geophysics Directorate,  
Hanscom AFB, MA  
<sup>1</sup>Stewart Radiance Laboratory, Bedford MA

Annual Review Conference on  
Atmospheric Transmission Models

June 1994

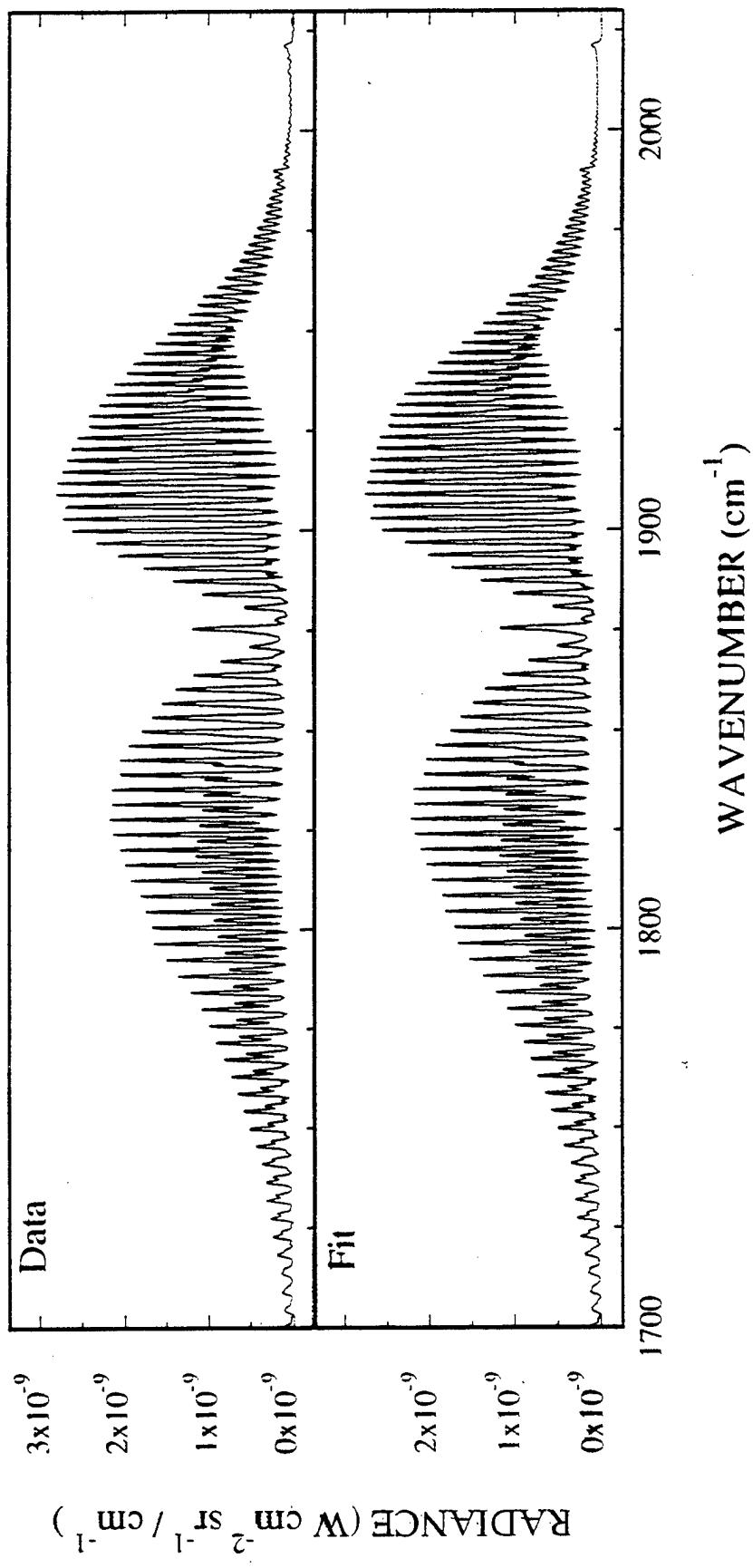
Supported by: Air Force Office of Scientific Research  
and the Ballistic Missile Defense Organization



# CIRRIS 1A EXPERIMENT



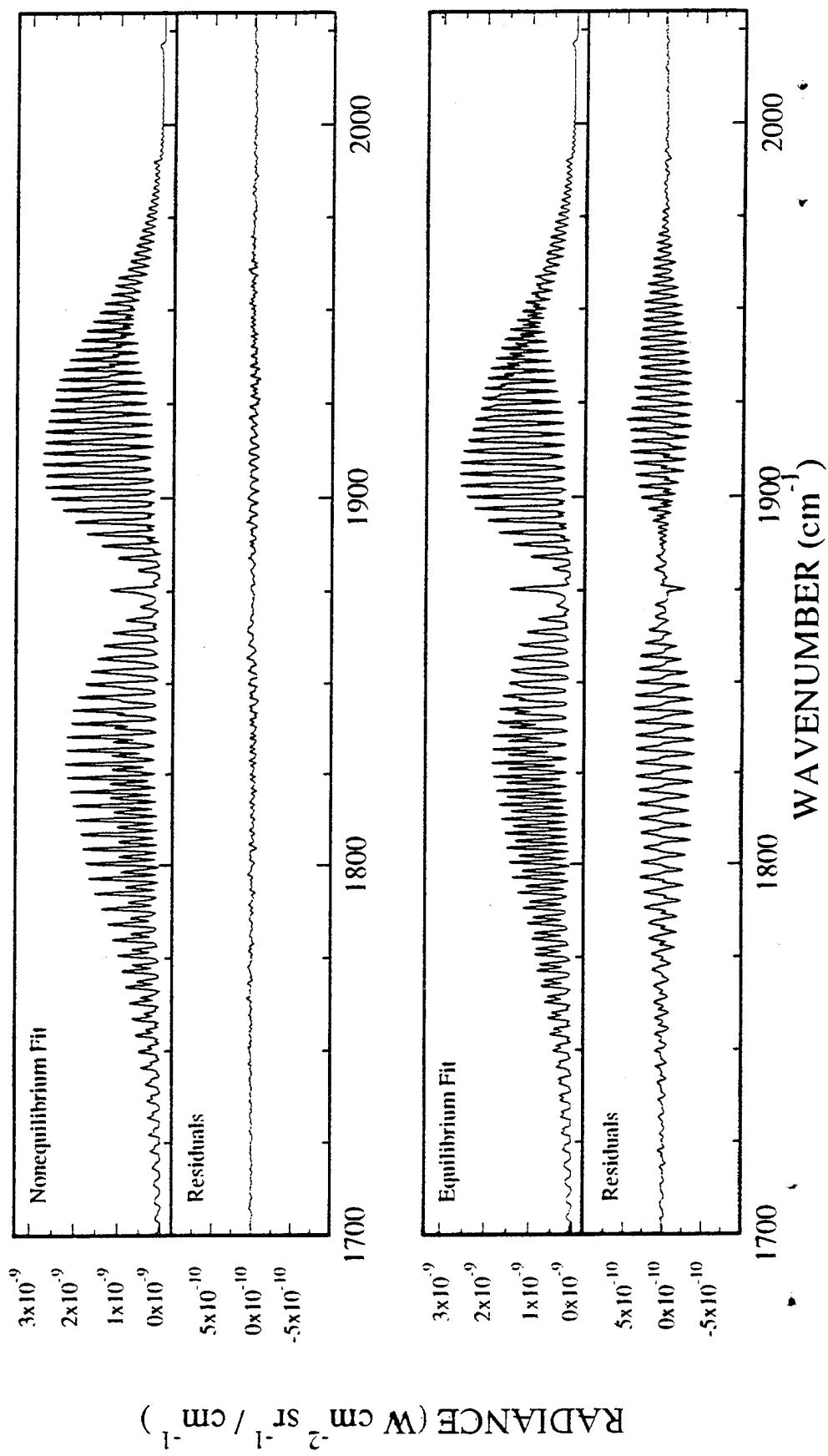
- High S/N earthlimb spectra recorded by Shuttle-based Michelson interferometer ( $1 \text{ cm}^{-1}$  resolution)
- Nitric oxide ( $^2\Pi_{\Omega}, \Omega = 1/2, 3/2$ )  $\Delta v = 1$  emissions



# Spectral Fits



- Nonequilibrium and equilibrium synthetic spectra
- Nonequilibrium fit matches spin-orbit features



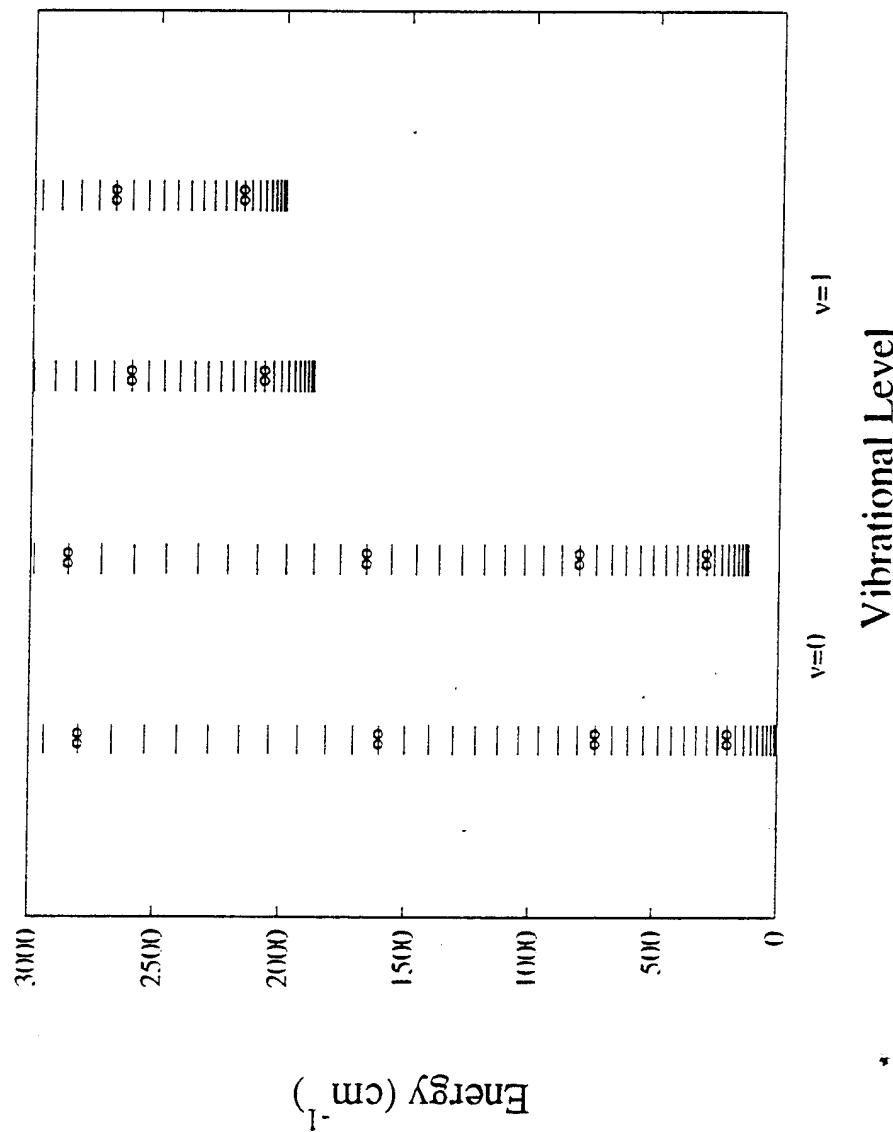
# Analysis of Subthermal Nitric Oxide Spin-Orbit Population Distributions

- Populations obtained by nonlinear synthetic spectral fitting
  - Spin-orbit equilibrium at T(rotation) gives large residuals
  - Best fit obtained for independent spin-orbit populations
- Large enhancement in lower spin-orbit manifold population
  - Energy separation between manifolds is only  $120 \text{ cm}^{-1}$
  - Effective spin-orbit temperature 200 K instead of 900 K
- Spin-orbit population enhancement increases with altitude
  - Collisional relaxation becomes dominant at lower altitudes
  - Limb view line-of-sight effects important below 135 km
- Trend of population ratio is consistent throughout data set
  - Much less variation seen than in radiance or temperature
  - Possible effect of chemical production seen in auroral data

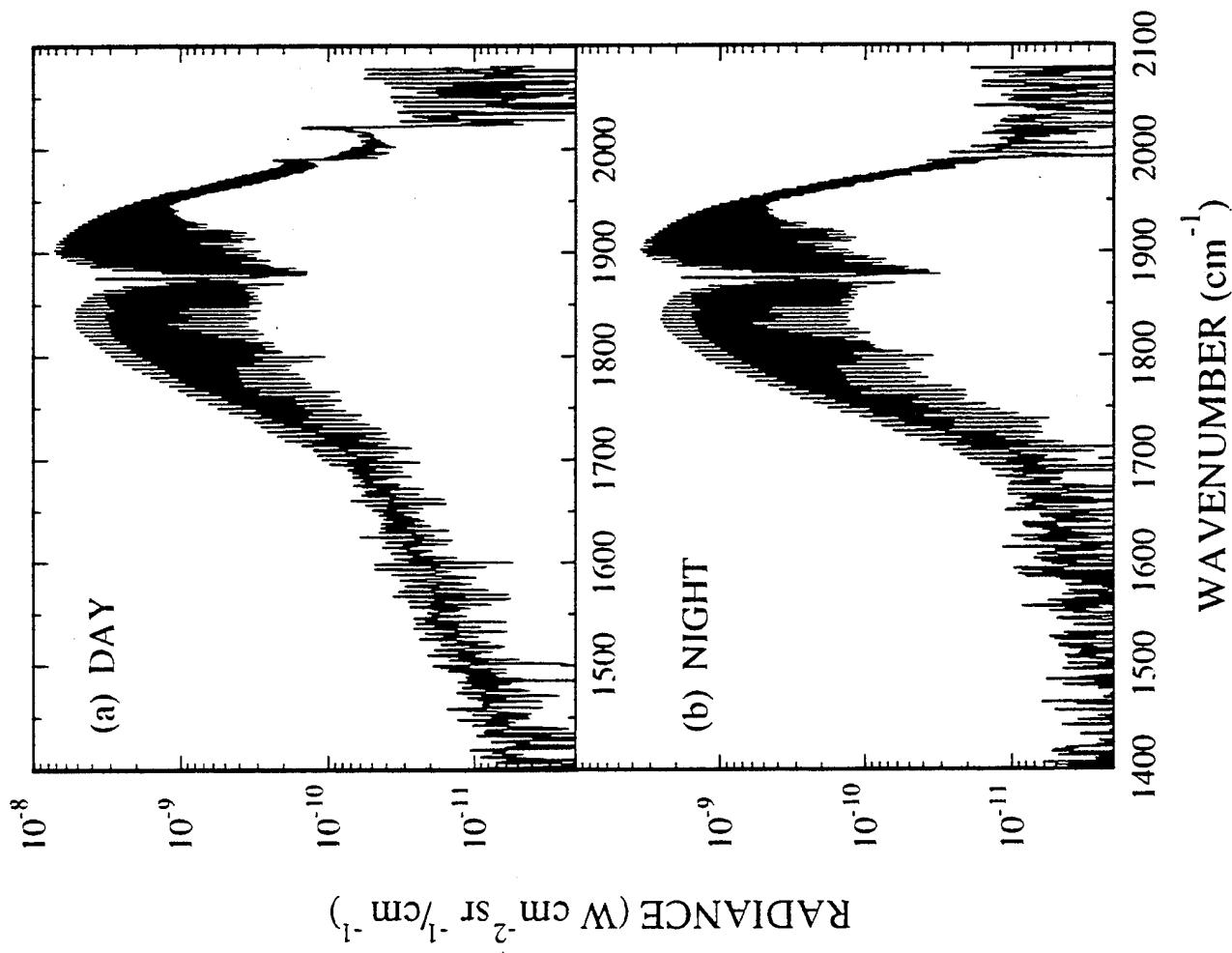


## Nitric Oxide Energy Level Diagram

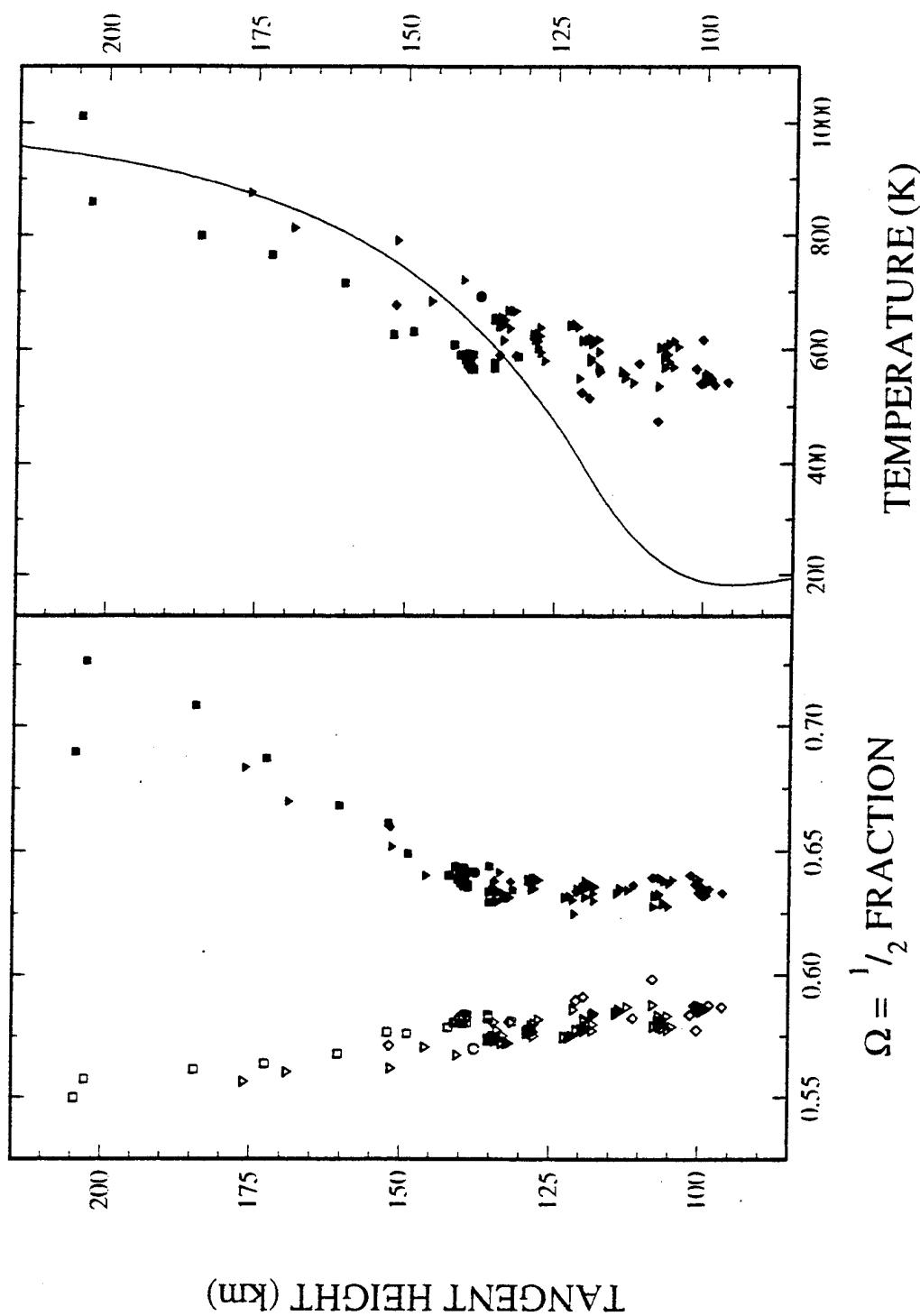
- Energies shown for the  $\Omega=1/2, 3/2$  spin-orbit manifolds for  $v = 0, 1$



# Daytime and Nighttime NO Spectra



# Spin-Orbit Altitude Profile



Expectation: open symbols  
Observation: filled symbols

MSIS Temperature Profile: line  
Observation: symbols

$$\Omega = \frac{1}{2} \text{ FRACTION}$$

TEMPERATURE (K)



## Origin of Subthermal Spin-Orbit Population Distribution

- Leading candidate is collisional uppumping by O atoms, main source of NO( $v=1$ ) in thermosphere
- Radiation, primary NO( $v=1$ ) loss mechanism, does not induce spin-orbit state preference
- Collisional relaxation occurs at insufficient rate at higher altitudes
- Chemical production has diurnal variation not observed in sublevel distributions



## Impact On Related Research

- Nonequilibrium OH sublevel distributions also observed in CIRRIS 1A experiment
- Subthermal NO sublevel distributions produced in laboratory  $\text{NO}_2$  photodissociation experiments
- Ground-based microwave measurements of NO densities in the upper atmosphere
- Band-integrated satellite measurements of NO radiance using pressure-modulated absorption
- Spin-orbit nonequilibrium must be taken into account when interpreting experimental data
- May provide method of discriminating chemical production from collisional up pumping in NO



**Comparison of Global Variations of the Radiance of  
the Stratospheric O<sub>3</sub>, CH<sub>4</sub> and HNO<sub>3</sub> Spectra as Viewed by  
CIRRIS 1A with UARS/CLAES Experiment.**

**B K Rezai<sup>1</sup>, G E Bingham<sup>2</sup>, L R Megill<sup>1</sup>, D K Zhou<sup>2</sup>, J L Mergenthaler<sup>3</sup>,  
A E Roche<sup>3</sup>, J B Kumer<sup>3</sup>, G P Anderson<sup>4</sup> and R D Nadile<sup>4</sup>**

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                         Utah State University, Logan, UT 84322-4405

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4                   Department of the Air Force, Phillips Laboratory (AFMC)/GPOS/GP  
                         Hanscom Air Force Base, Massachusetts 01731-3010

**PRESNTED TO 17TH ANNUAL REVIEW CONFERENCE ON  
ATMOSPHERIC RADIATION MODELS  
HANSCOM AFB, MA  
JUNE 7, 1994**

## ABSTRACT

The importance of the distribution of  $O_3$ ,  $CH_4$  and nitrogen compounds to stratospheric chemistry has been clearly established. We report on measurements of these species by the Cryogenic Infrared Radiation Instrumentation for Shuttle (CIRRIS 1A) which flew aboard Discovery OV-103, (STS-39) on April 28 to May 6, 1991. By looking in the limb, it was possible to obtain approximately a thousand interferograms. This made possible the identification of many important stratospheric gases, including  $O_3$ ,  $CH_4$ ,  $HNO_3$  and chlorine source species  $CCl_2F_2$  and  $CCl_3F$ . The accuracy of the CIRRIS 1A measurements is therefore of interest in polar ozone depletion studies, and validation is a major consideration. This paper reviews the CIRRIS 1A observations of  $O_3$ ,  $CH_4$  and  $HNO_3$  spectra and deduced vertical profile concentrations, discusses their accuracy and precision. We compare the CIRRIS 1A measurements with the Cryogenic Limb Array Etalon Spectrometer (CLAES) on board the Upper Atmosphere Research Satellite. Specifically we compare CIRRIS 1A and CLAES spectra in the wavelength regions targeted for  $O_3$ ,  $CH_4$  and  $HNO_3$  concentration retrievals, and we compare the retrieved quantities for species in the southern and northern hemispheres. Since CIRRIS 1A data were collected shortly before, and CLAES data shortly after, the Pinatubo eruption, such comparisons are of significant value both scientifically and from a validation standpoint.

## CLAES - CIRRIS 1A OVERVIEW FOR CORRELATIVE STUDY

We discuss data from CLAES on the UARS satellite which viewed the stratospheric observations for over 19 months beginning in October 1991.

CLAES narrow band channels of the blocker filters regions 8, 6, and 4 (centered at wavenumbers of  $792 \text{ cm}^{-1}$ ,  $879 \text{ cm}^{-1}$  and  $1257 \text{ cm}^{-1}$ ) were used to retrieve  $\text{O}_3$ ,  $\text{HNO}_3$  and  $\text{CH}_4$  profiles. A multi-channel, multi-emitter retrieval scheme is used to establish the VMR [Roche et al, 1993].

CLAES spectral emission radiance measurements for a range of altitudes and their components are examined. These examples will illustrate instrument continuous scan mode spectral regions and their performance.

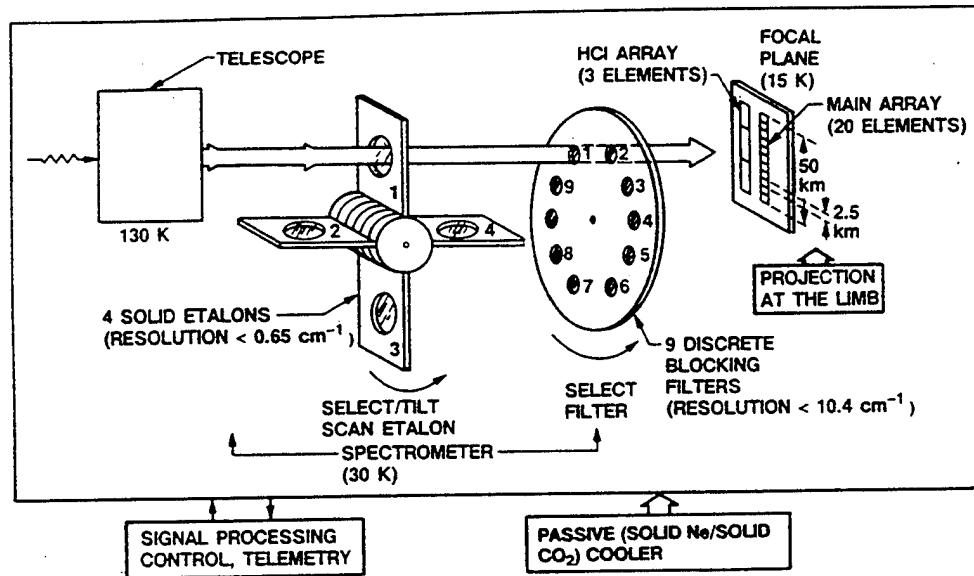
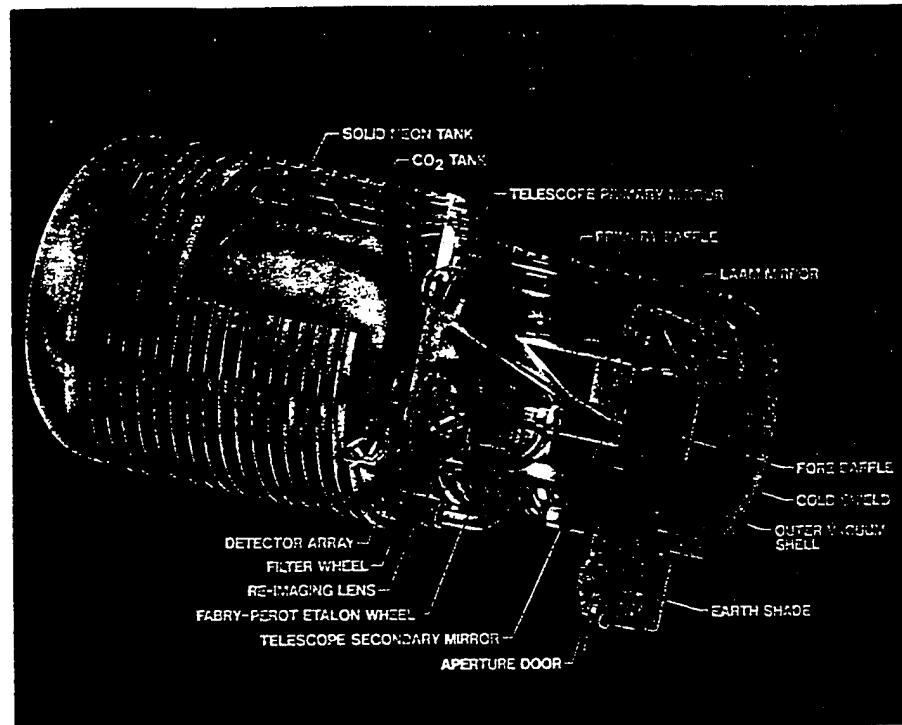
## CLAES - CIRRIS 1A OVERVIEW FOR CORRELATIVE STUDY COUNT.

We also discuss an analysis of the measurements obtained from the CIRRIS 1A payload aboard the STS-39, that viewed the stratosphere on April 28 to May 6, 1991.

The CIRRIS 1A payload consists of the two primary sensors (cryogen-cooled radiometer and interferometer), and co-aligned ancillary sensors, mounted to a two-axis gimbal system. The Interferometer is a Michelson design and features a flex-pivot mirror translation system.

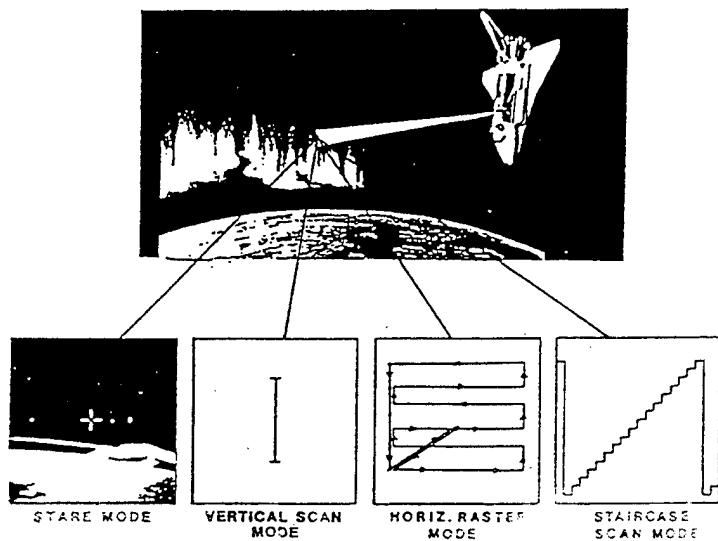
The interferometer focal plane contains five Si:AS detectors behind an eight-position filter wheel that respond to radiation between 2.5 and 25 microns and provides a spectral resolution ranging between  $1\text{ cm}^{-1}$  and  $8\text{ cm}^{-1}$  over an eight-order dynamic range [Coney et al, 1992].

# CLAES DESIGN AND FUNCTIONAL DIAGRAM

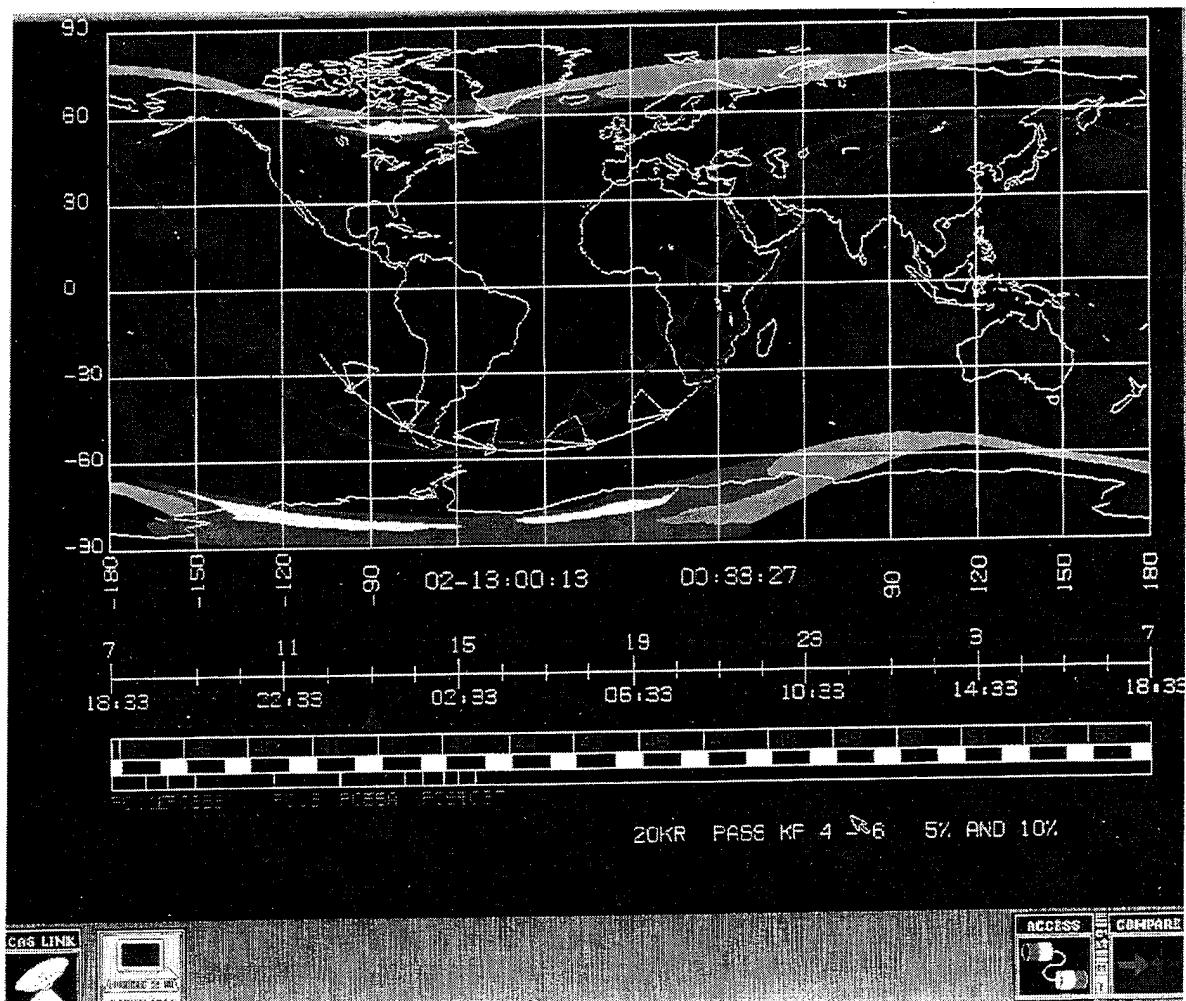


\*See Roche et al.

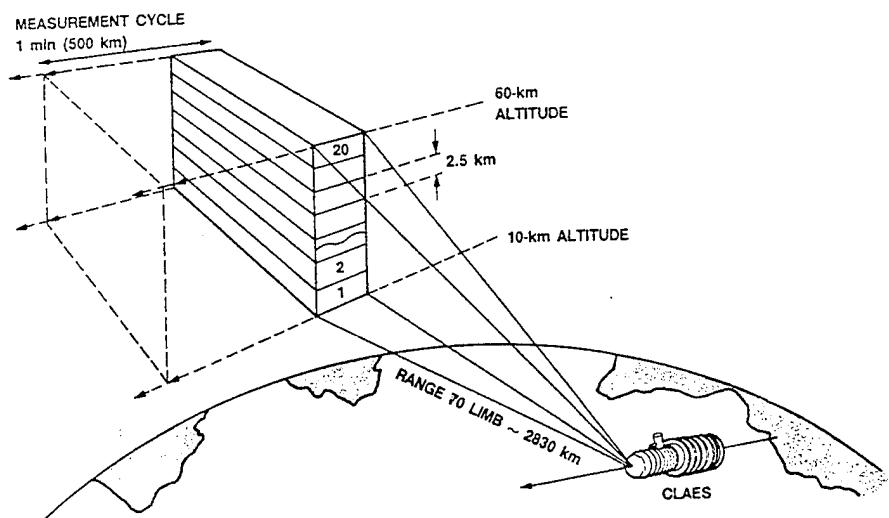
JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 98, NO. D6, PAGES 10,763-10,775,  
JUNE 20, 1993



CIRRIS 1A viewing & illustration of gimbal motion for typical mode  
 [Bartschi B. et al, 1987]

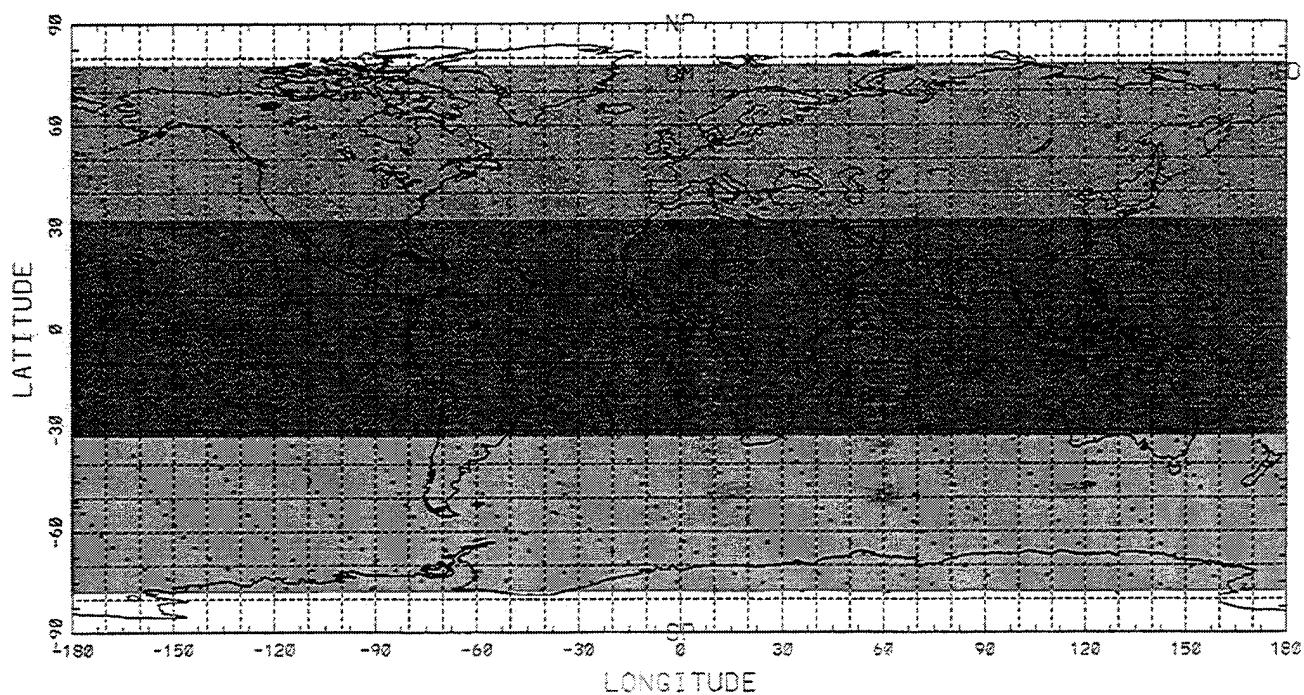


Typical course of the Shuttle during STS-39 flight for April 28 and May 6, 1991. Photograph shows CIRRIS 1A orbit and typical look angles and projected auroral intensity and locations. A portion of the CIRRIS 1A flight was dedicated to stratospheric gas measurements. Courtesy of USAF Phillips Laboratory and Radex, INC.



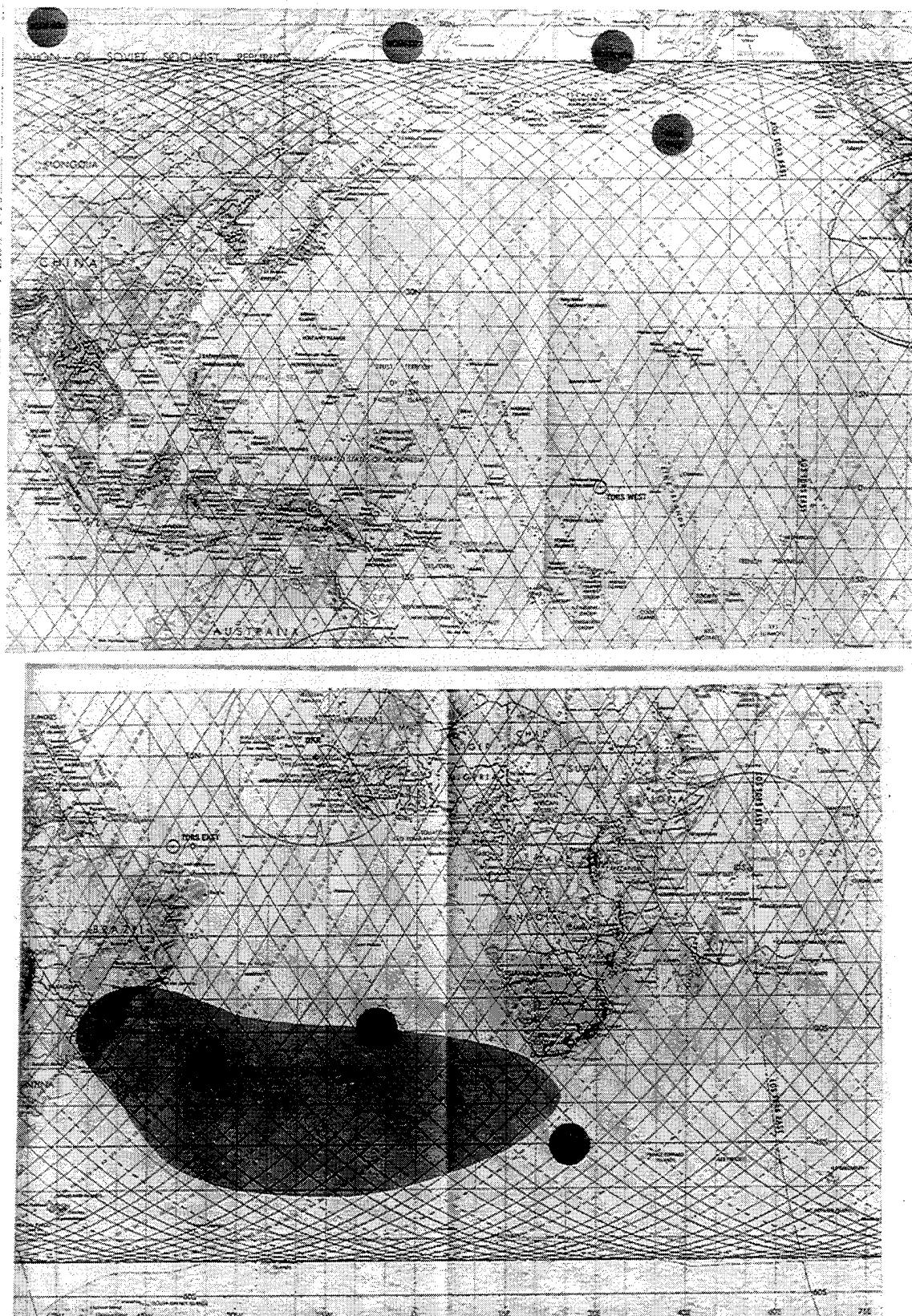
CLAES viewing geometry [Roche et al, 1993]

### CLAES NORTH-SOUTH LOOKING COVERAGE DURING STRATOSPHERIC GAS MEASUREMENTS



CLAES latitude versus longitude coverage for the month of April 1992. Points at which calibrations were performed for each descending day are shown. Violet indicates north looking; aqua indicates south looking; blue is the overlap regions. Upper and lower panels each contain about 600 data points from 16 orbits over a 24 hour period covering any latitude band.

## SHUTTLE GROUND TRACK DURING STRATOSPHERIC GAS MEASUREMENTS



Typical course of the Shuttle during STS-39 flight for April 28 and May 6, 1991. A portion of the CIRRIS 1A flight was dedicated to stratospheric gas measurements. Points indicate seven data sampling profiles locations.



# CALCULATED RADIANCE AT THE SENSOR FOR LIMB TANGENT ALTITUDE $h$ , FREQUENCY $\nu_i$

Lockheed

$$R_i(h, \nu_i) = - \int_{\nu_1}^{\nu_2} \int_{\phi_1}^{\phi_2} \int_{s=0}^{\infty} B(\nu_i, T) F(\phi) R(\nu_i) \frac{d\tau_i(\nu s)}{ds} d\nu d\phi ds$$

PLANCK FUNCTION AT  $\nu_i$ , T, POINT S

INSTRUMENT SPATIAL RESPONSE FUNCTION

INSTRUMENT SPECTRAL RESPONSE FUNCTION AT  $\nu_i$

DERIVATIVE OF TRANSMITTANCE FROM POINT S TO SENSOR

WHERE

$$\tau_i = \exp \left[ - \int_s^{\infty} k_r(P, T) q \, ds \right]$$

AND

$$K_r(P, T) = \frac{S\alpha}{\pi[(\nu - \nu_0)^2 + \alpha^2]} = \text{SPECTRAL ABSORPTION CROSS SECTION FOR LORENTZ LINE SHAPE}$$

THE MEASURED RADIANCE IS OBTAINED AS

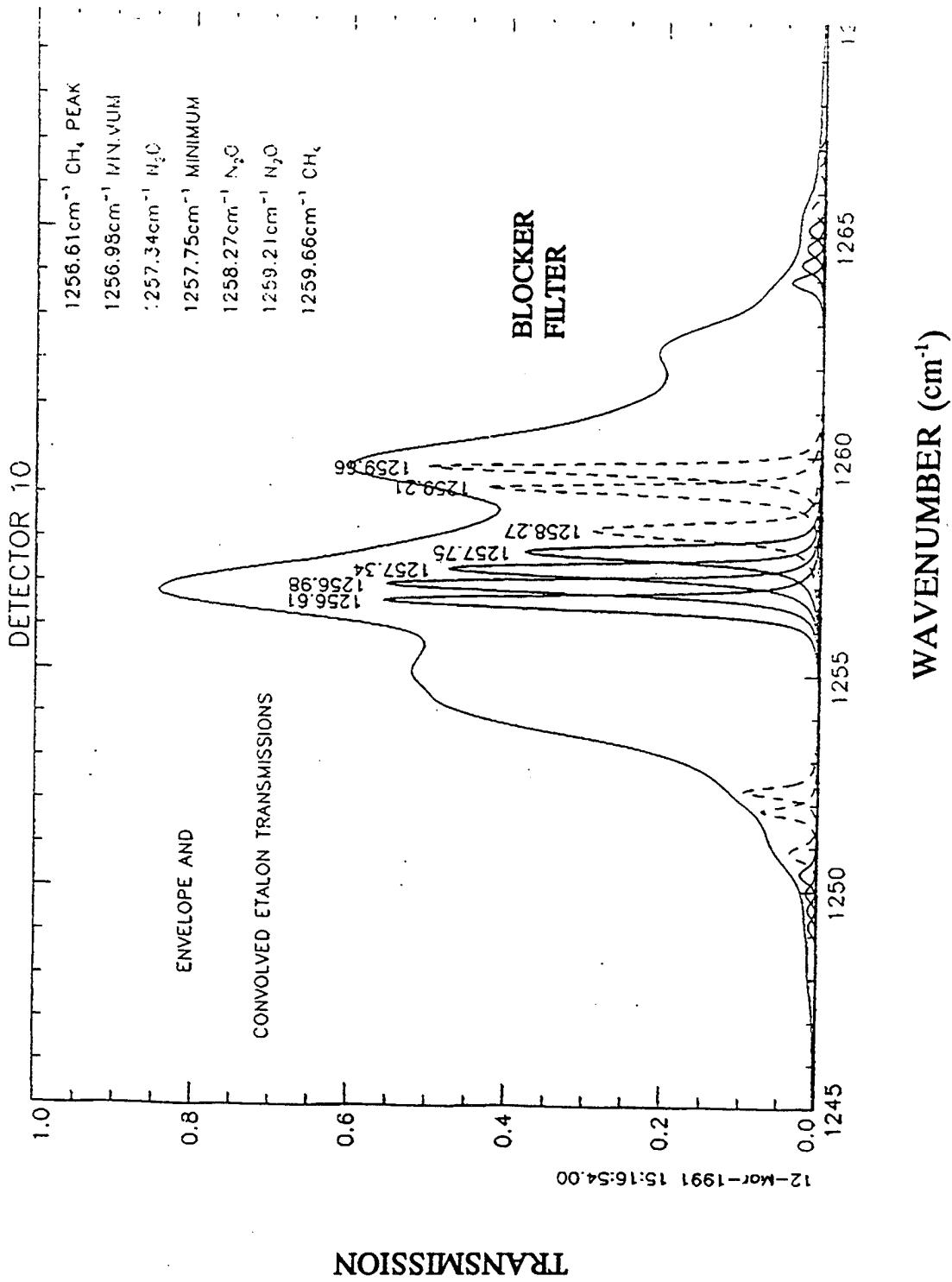
$$N_i(h, \nu_i) = D_i (\text{VOLTS}) \times \text{CAL}_i (\text{RADIANCE/VOLTS})$$

BY COMPARING ALL  $R_i$  AND  $D_i$  FOR EACH TANGENT ALTITUDE, SOLUTIONS ARE FOUND BY ITERATING  $T$ ,  $P$ , AND  $q$

X90907\_R\_JS\_LC

X90907\_R\_JS\_LC

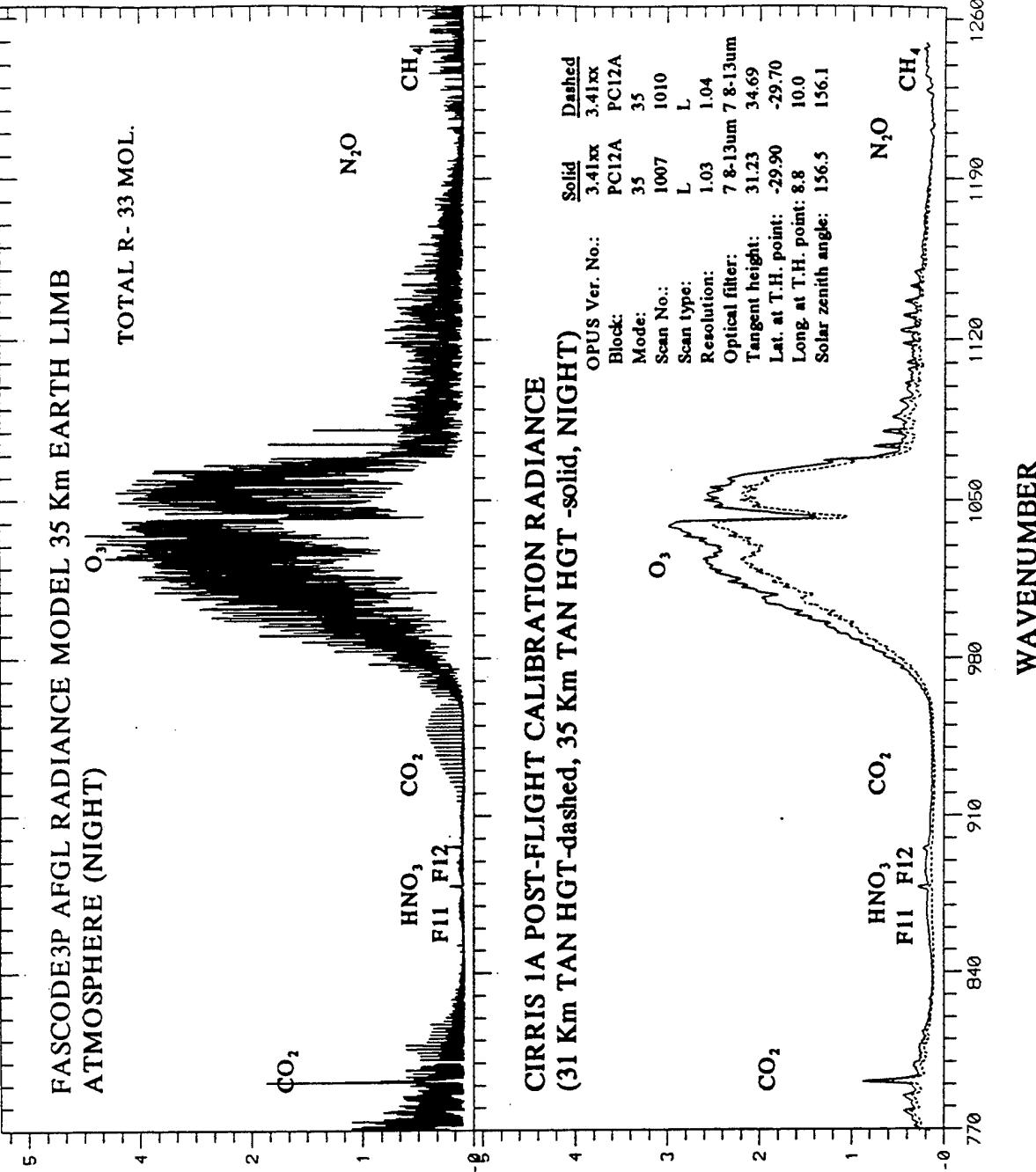
## CLAES ETALON AND BLOCKER FILTER



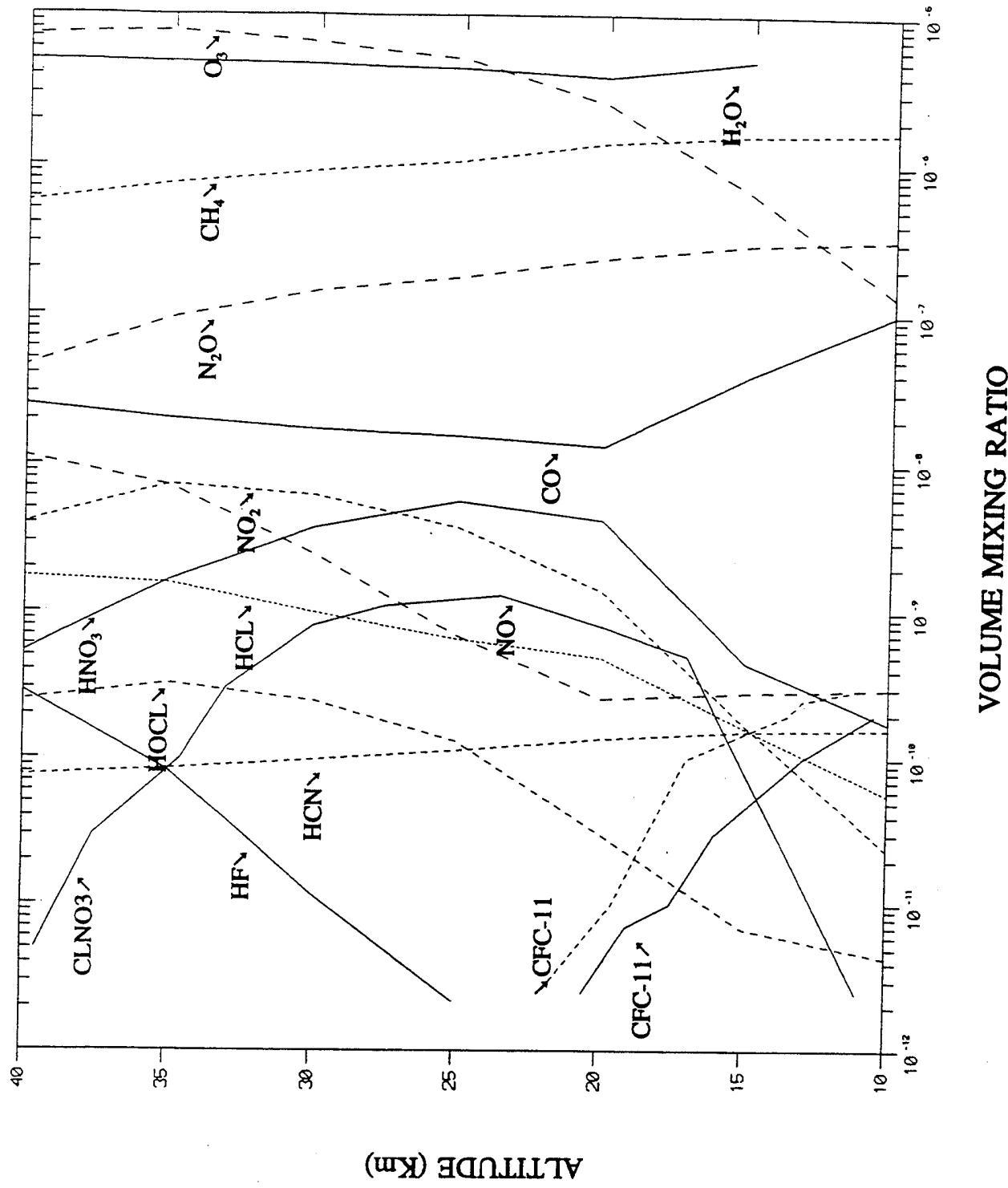
Example of CLAES blocker etalon transmittances for Etalon tilt positions for blocker filter region 4.

# CIRRIS 1A INFRARED AND ATMOSPHERIC RADIATION MODEL

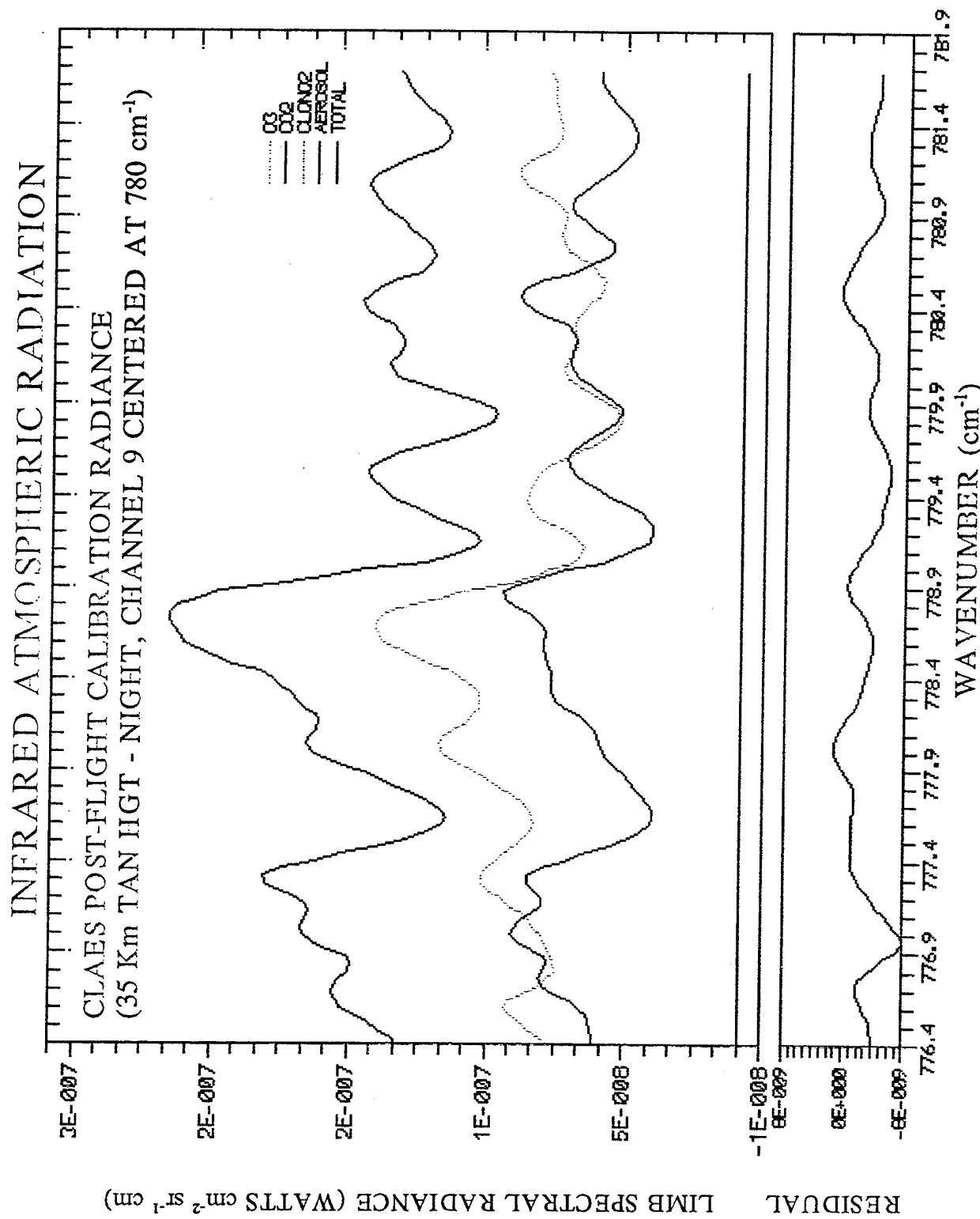
LIMB SPECTRAL RADIANCE (WATTS  $\text{cm}^{-2} \text{sr}^{-1} \text{ cm}^{-1}$ )  $\times 10^6$



The spectral distribution of infrared emission produced by minor species in the stratosphere. The figure compares the AFGL radiance model (FASCODE3P line-by-line radiation code), with data taken by the Cryogenic Infrared Radiance Instrumentation for Shuttle (CIRRIS 1A) viewing the earth limb at altitudes of 31 and 35 km.



VMR profiles used in the analysis of mid-latitude spectra over the southern hemisphere.



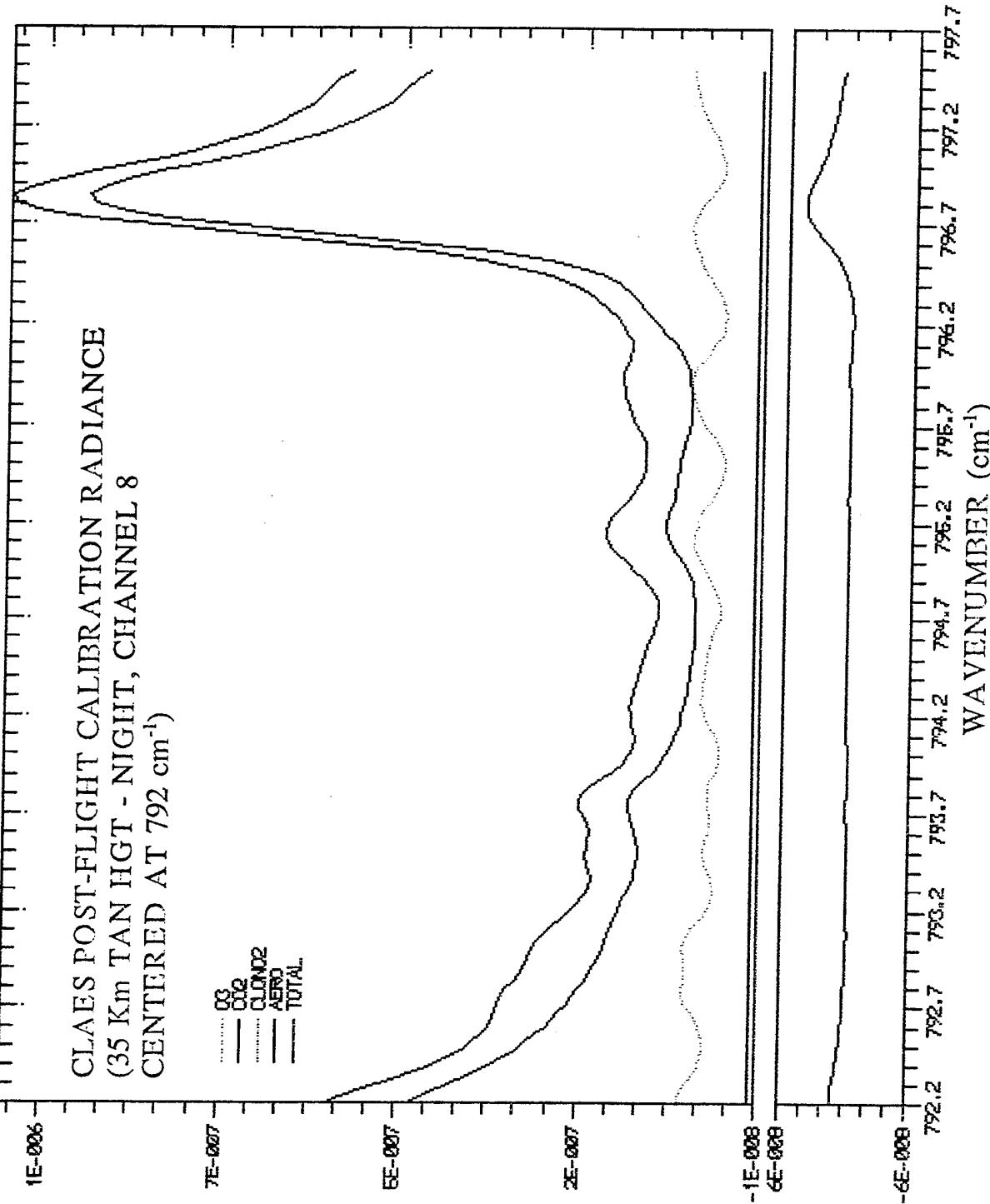
The spectral distribution of infrared emission produced by minor species in the stratosphere. The figure shows the spectral emissions measured by the Cyrogenic Array Etalon Spectrometer (CLAES) viewing the earth limb at altitude of 35 km.

# INFRARED ATMOSPHERIC RADIATION

CLAES POST-FLIGHT CALIBRATION RADIANCE  
 (35 Km TAN HGT - NIGHT, CHANNEL 8  
 CENTERED AT  $792 \text{ cm}^{-1}$ )

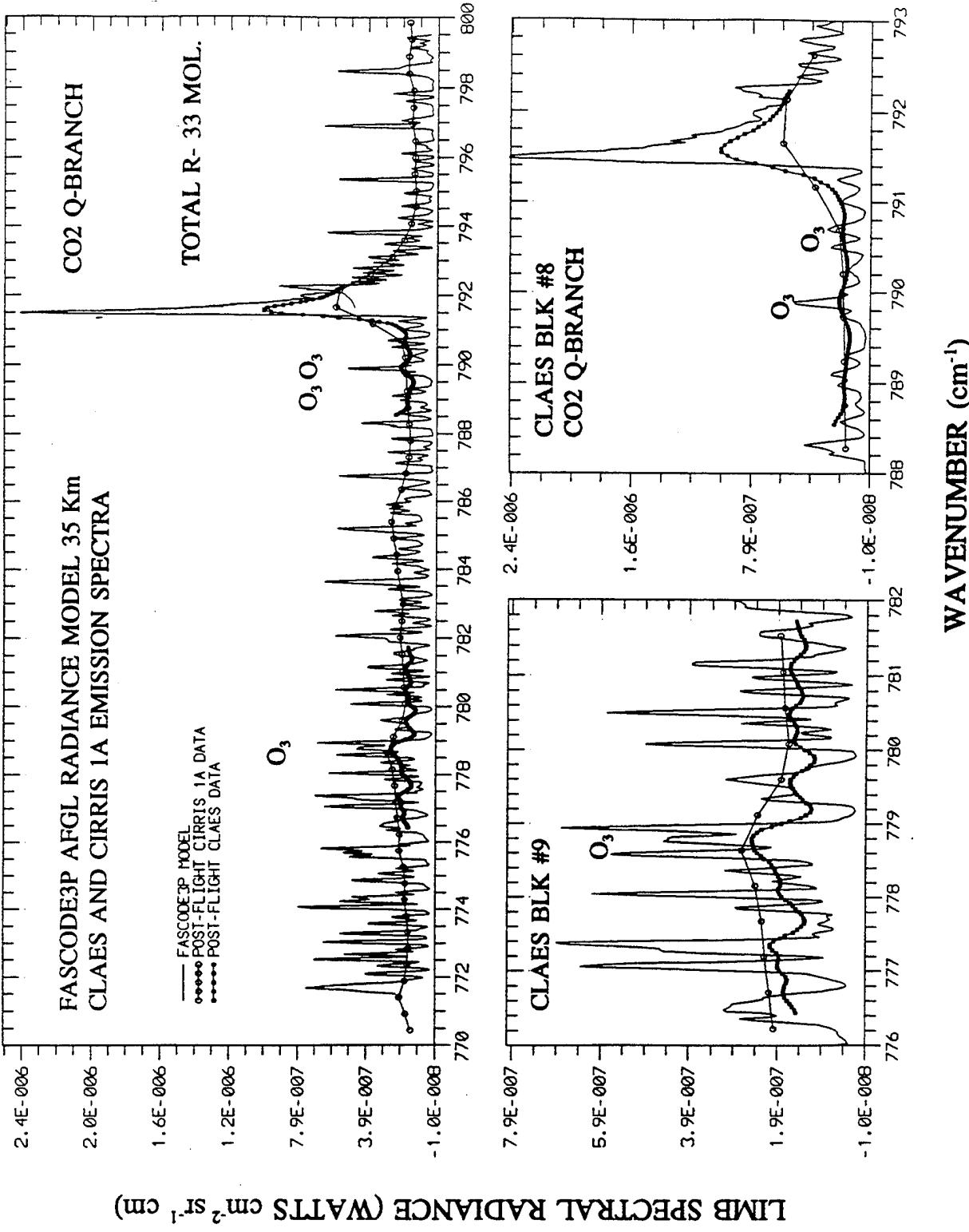

 O<sub>3</sub>  
 CO<sub>2</sub>  
 AERO  
 TOTAL

RESIDUAL      LIMB SPECTRAL RADIANCE (WATTS  $\text{cm}^{-2} \text{sr}^{-1} \text{cm}^{-1}$ )



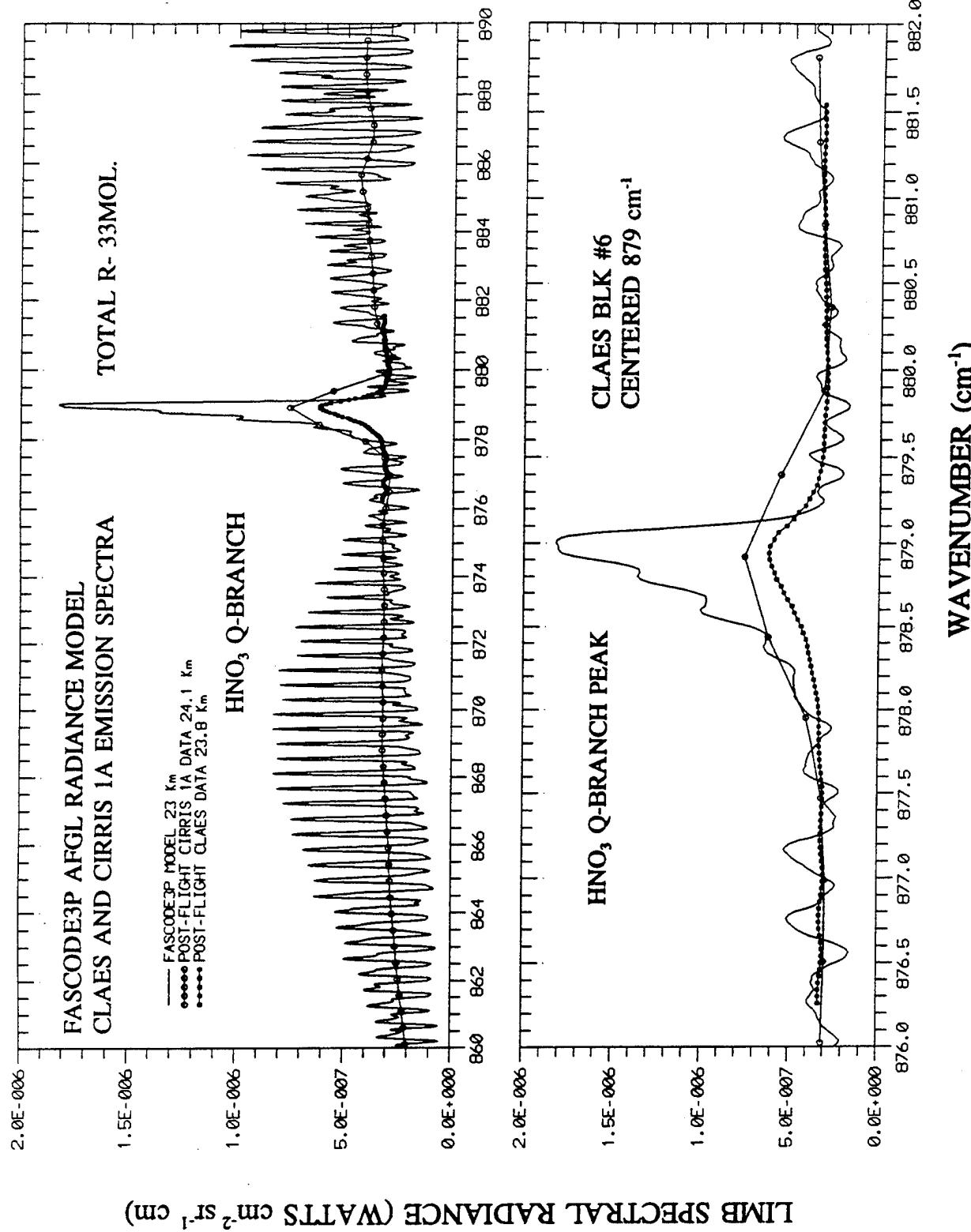
The spectral distribution of infrared emission produced by minor species in the stratosphere. The figure shows the spectral emissions measured by the Cryogenic Array Etalon Spectrometer (CLAES) viewing the earth limb at altitude of 35 km.

# CLAES, CIRRIS 1A DATA AND RADIATION MODEL COMPARISONS



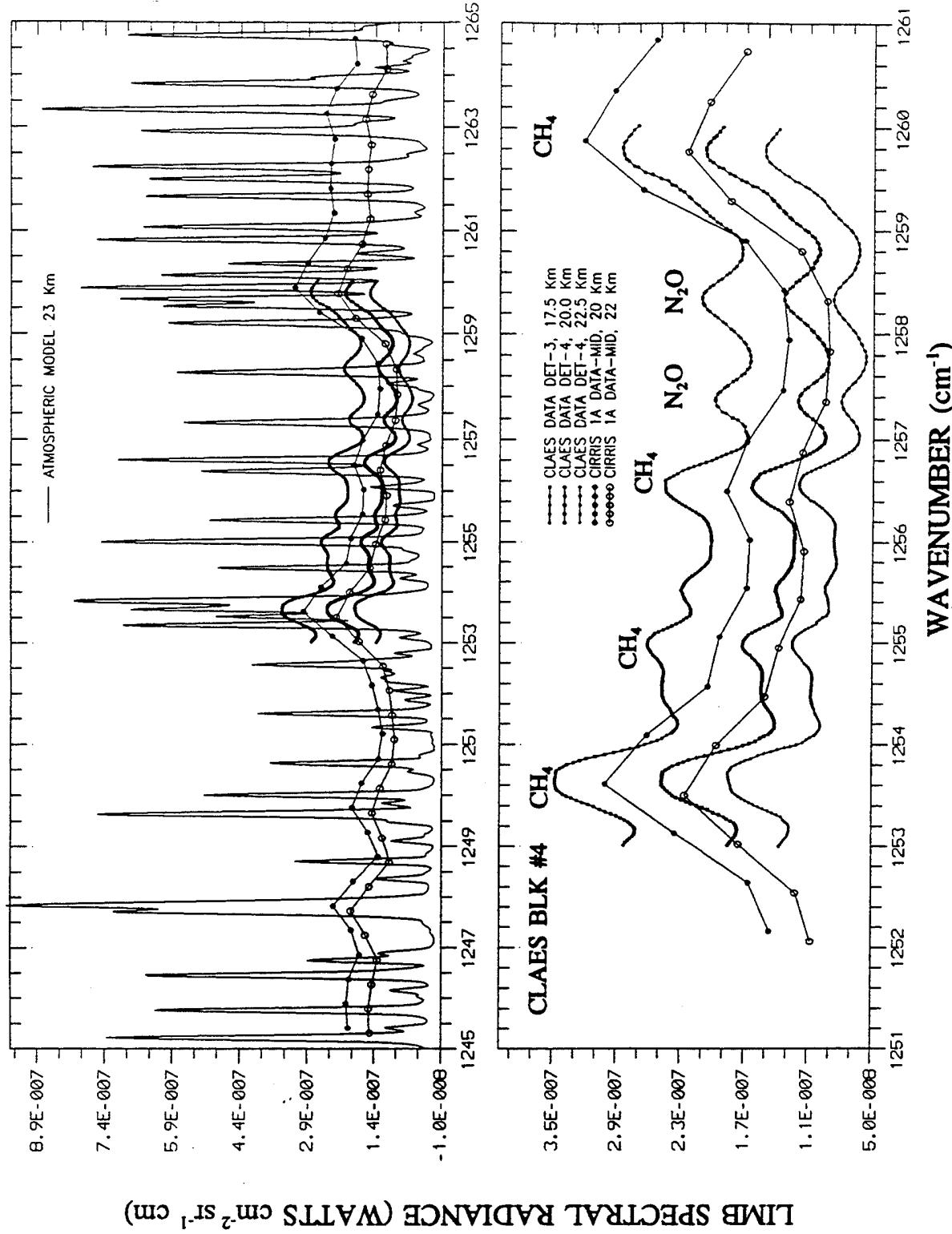
Correlation and anti-correlation between CLAES, CIRRIS 1A O<sub>3</sub> data compared with FASCODE3P model.  
The figure shows that the line position, intensity and spectral distributions measured by CLAES and CIRRIS 1A agree with each other and with those of the model at this altitude.

# CLAES, CIRRIS 1A DATA AND MODEL COMPARISONS



CLAES and CIRRIS 1A HNO<sub>3</sub> spectra compared with model at 23 Km tangent height. The figure shows the measured and model spectra agree quite well. The model spectral resolution is 0.02  $\text{cm}^{-1}$ . When intercomparing the residual spectra, the slightly different scaling should be regarded.

# CLAES, CIRRIS 1A DATA AND RADIATION MODEL COMPARISONS



Correlation between CLAES, CIRRIS 1A  $\text{CH}_4/\text{N}_2\text{O}$  data compared with line-by-line model radiation.

## SUMMARY

We have presented the analysis of CLAES spectral emission measured data and CIRRIS 1A interferometric data.

Data from the CIRRIS 1A interferometer and the CLAES spectral emission measurements (and their components of the computed fit) were used to characterize the O<sub>3</sub>, HNO<sub>3</sub> and CH<sub>4</sub> emission.

Forward calculations of spectra were performed by the FASCODE3P line-by-line radiation code. The code was modified in order to permit the calculation of CFC's and ClONO<sub>2</sub> emissions from absorption cross-sections.

Our study of CLAES-CIRRIS 1A spectra shows that the line positions, intensity, and spectral distribution agree with each other and with those of the model at selected altitude and latitude to within experimental accuracy.

## SUMMARY COUNT.

This line of investigation appears to be very promising for comparison of the techniques but more work is necessary establish additional information.

The integrated radiances of selected spectral features, are used to infer the concentration profiles of some atmospheric constituents including chlorine containing sources (CFC-11, CFC-12) as well as HNO<sub>3</sub>, O<sub>3</sub>, CH<sub>4</sub>.

This presentation of stratospheric gas measurements for CLAES spectral emission and CIRRIS 1A interferometric data is preliminary. There is a wealth of excellent spectra that need to be reduced, analyzed, correlated and interpreted.

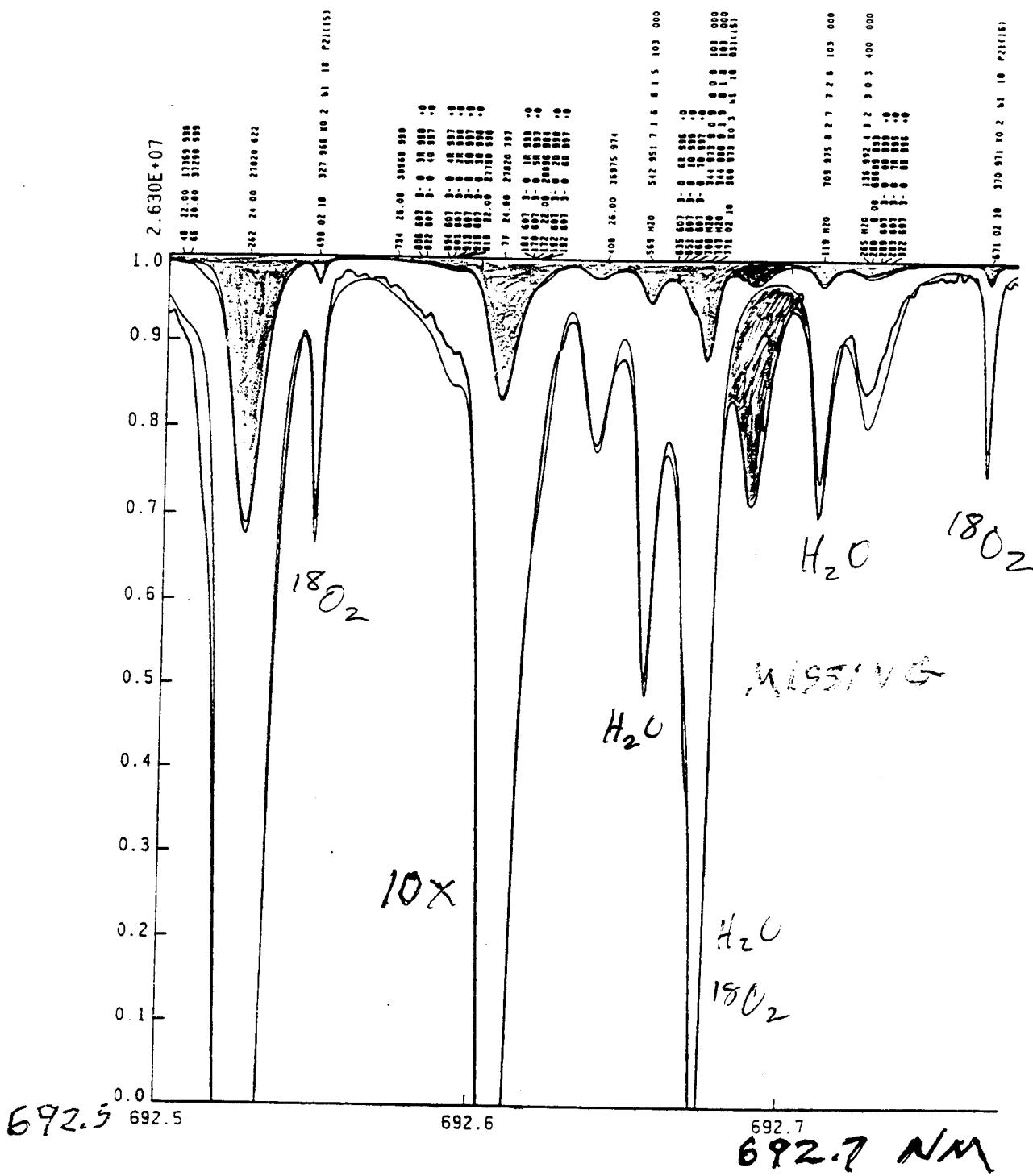


Fig. 1. A small section of solar central intensity spectrum at 692.5 nm plotted at full scale and at 10 times scale. The heavy lines are the observed FTS spectrum from James Brault at Kitt Peak. The resolution is 522000 and the signal-to-noise is about 3000 which is poor for this work. The continuum level is uncertain. The thin line is the computed spectrum. It would be possible to adjust the line data for a better match but most of the discrepancies are from missing lines. There are solar lines of Ca I, Ti I, Cr I, Fe I, C I, CN, and terrestrial lines of H<sub>2</sub>O and <sup>16</sup>O<sup>18</sup>O. The first number in each line label is the last 3 digits of the wavelength and the 4th number is the per mil central intensity if the line were computed in isolation.

Annual Review Conference on Atmospheric Transmission Models  
7-8 June 1994, Phillips Laboratory, Bedford, MA

## The POAM II Experiment and Early Measurement Results

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**Eric Chassefière, Francis Dalaudier, & Carole Deniel**  
Service d'Aéronomie du CNRS

**Jacqueline Lenoble & Collette Brogneiz**  
Université de Science et Technologie de Lille

**David Rusch, Todd Clancy, & Cora Randall**  
University of Colorado

**John Olivero**  
Embry-Riddle Aeronautical University

## *Polar Ozone and Aerosol Measurement (POAM II) Science Summary*

*POAM II uses proven visible solar occultation and techniques  
from a polar orbiting spacecraft - SPOT 3.*

*The solar occultation technique consists of measuring solar extinction as a function of frequency as the sun rises or sets relative to the spacecraft. From these measurements the abundance profile of absorbing gases and aerosol extinction profiles can be determined.*

*POAM II measures key constituents of the polar stratosphere:  
aerosols, O<sub>3</sub>, H<sub>2</sub>O, NO<sub>2</sub>, and temperature.*

*POAM II measurements are vital to understanding the Antarctic "ozone hole" and possible development of Arctic ozone depletions.*

## **POAM II - (Polar Ozone & Aerosol Measurement)**

### **9 Channel Solar Occultation Instrument launched on the SPOT 3 Satellite**

- Designed to measure long-term trends in ozone abundances at polar latitudes, and examine the morphology of spring-time ozone depletions in the polar regions.
- Measure stratospheric aerosol extinction profiles and obtain a climatology of Polar Stratospheric Clouds (PSC's).
- Make zonal average measurements of H<sub>2</sub>O and NO<sub>2</sub> in the stratosphere.
- Make observations of the frequency of occurrence and optical thickness of high cirrus clouds.



## OPTICAL HEAD ASSEMBLY

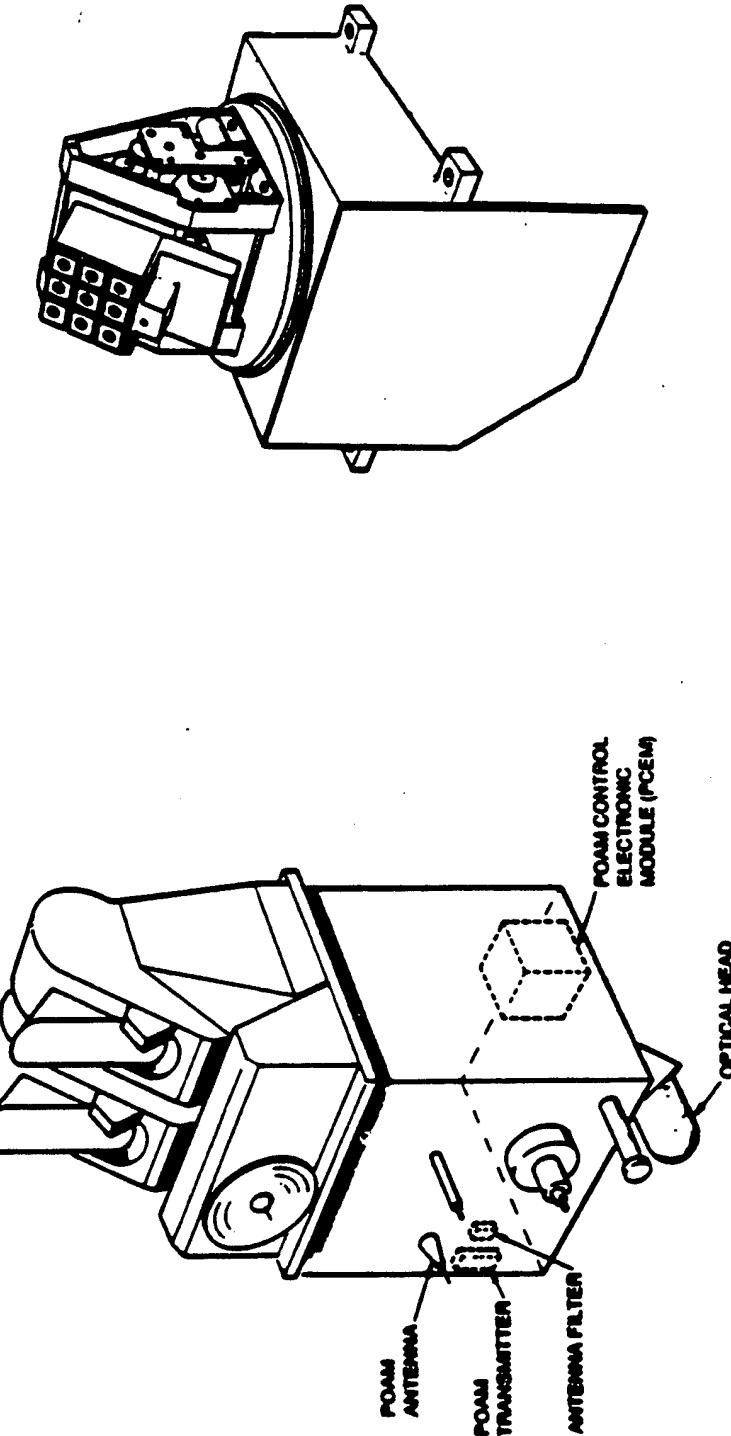
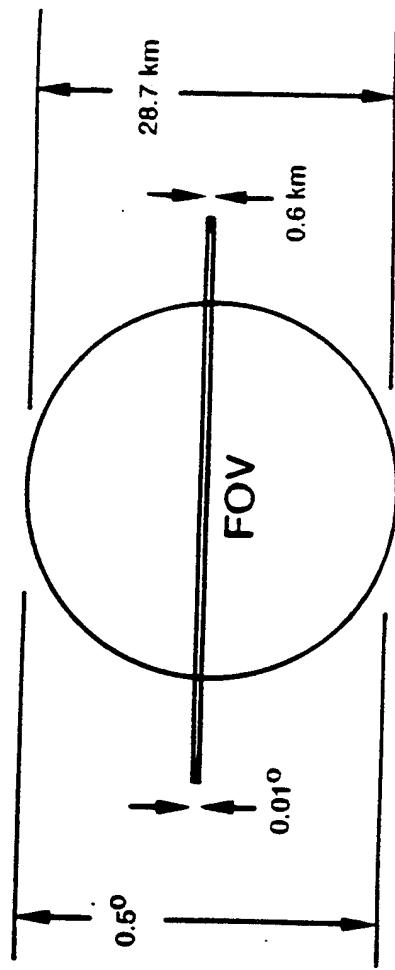
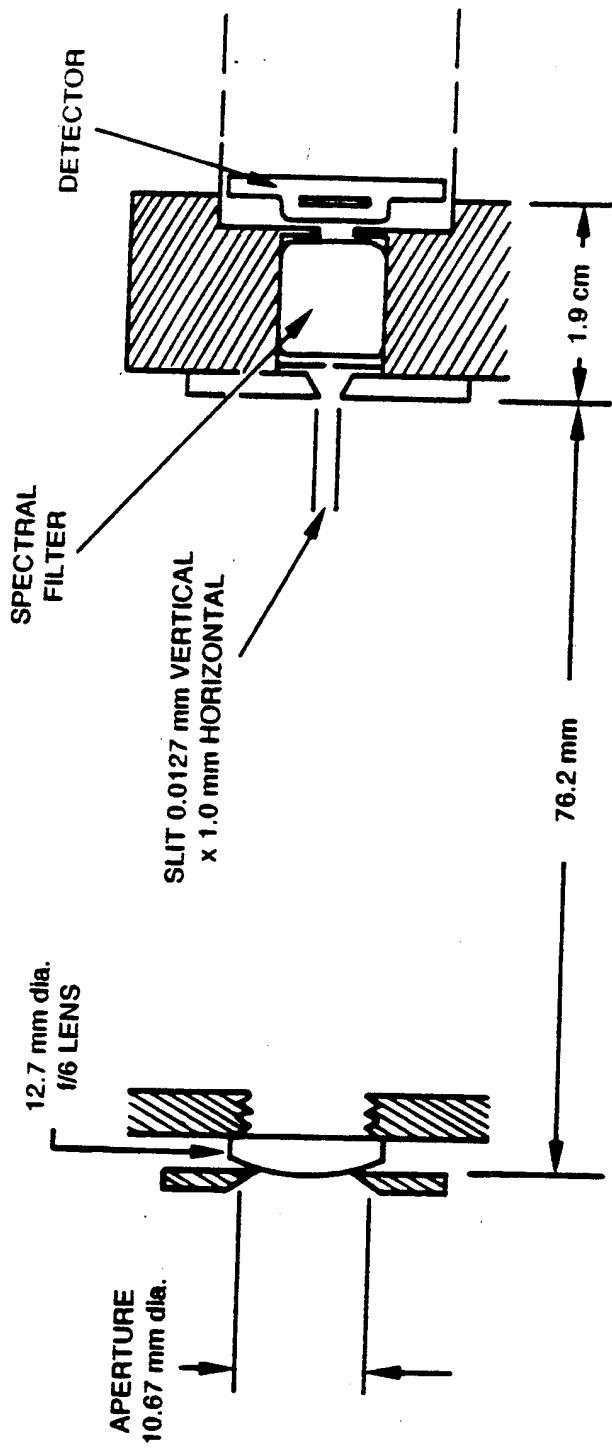


Figure 1: Schematic drawing showing the location of the POAM II instrument components integrated onto the SPOT 3 satellite (left) and schematic of the POAM II Optical Head Assembly (right).

# SCIENCE SENSORS OPTICAL PATH



**FOV defined by lens to slit distance and slit width**

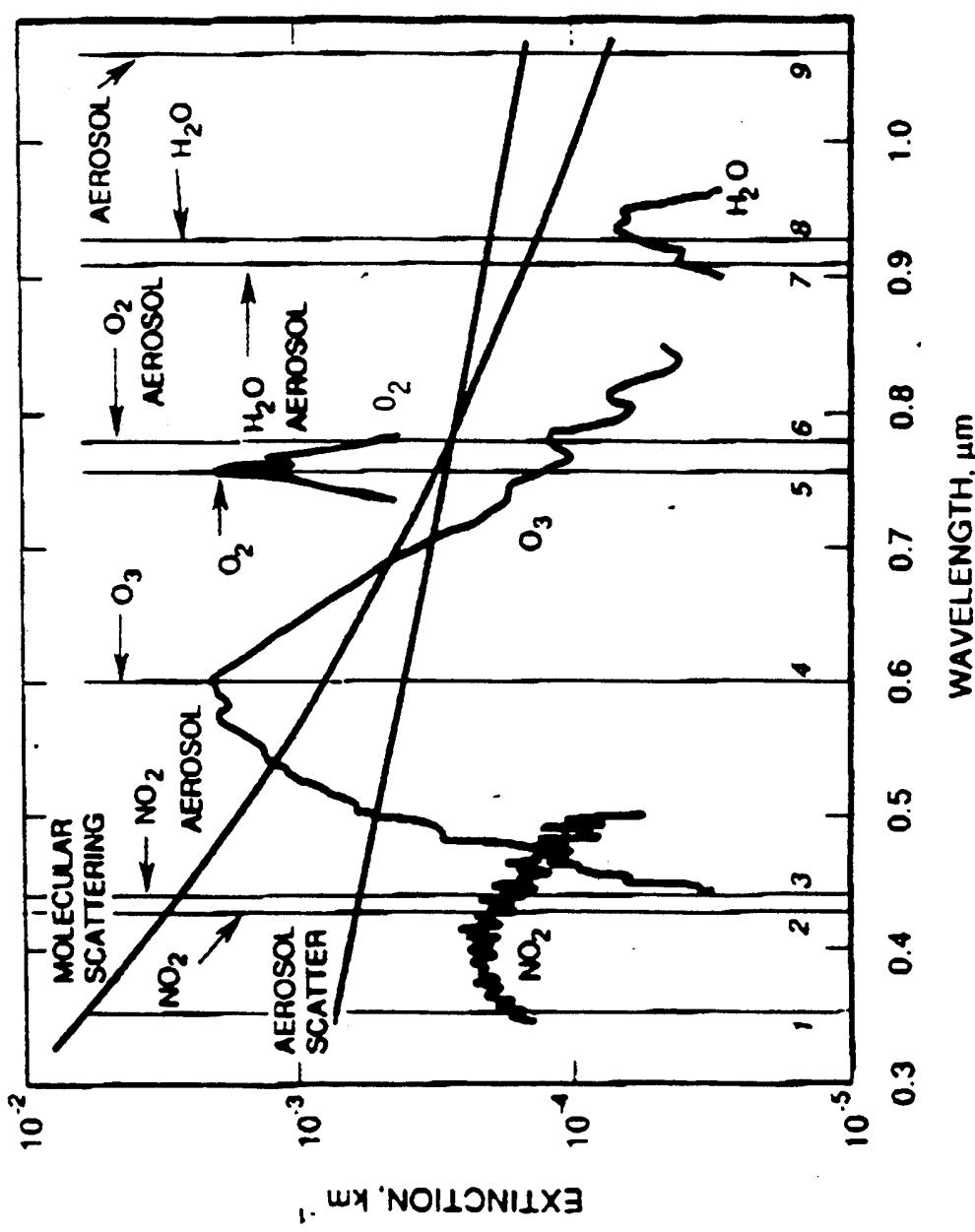
$$\text{FOV} = 0.01^\circ \times 0.76^\circ$$

$$\begin{aligned} \text{Pointing stability} &= 0.005^\circ \text{ (vert.)} \\ &= 0.05^\circ \text{ (hor.)} \end{aligned}$$

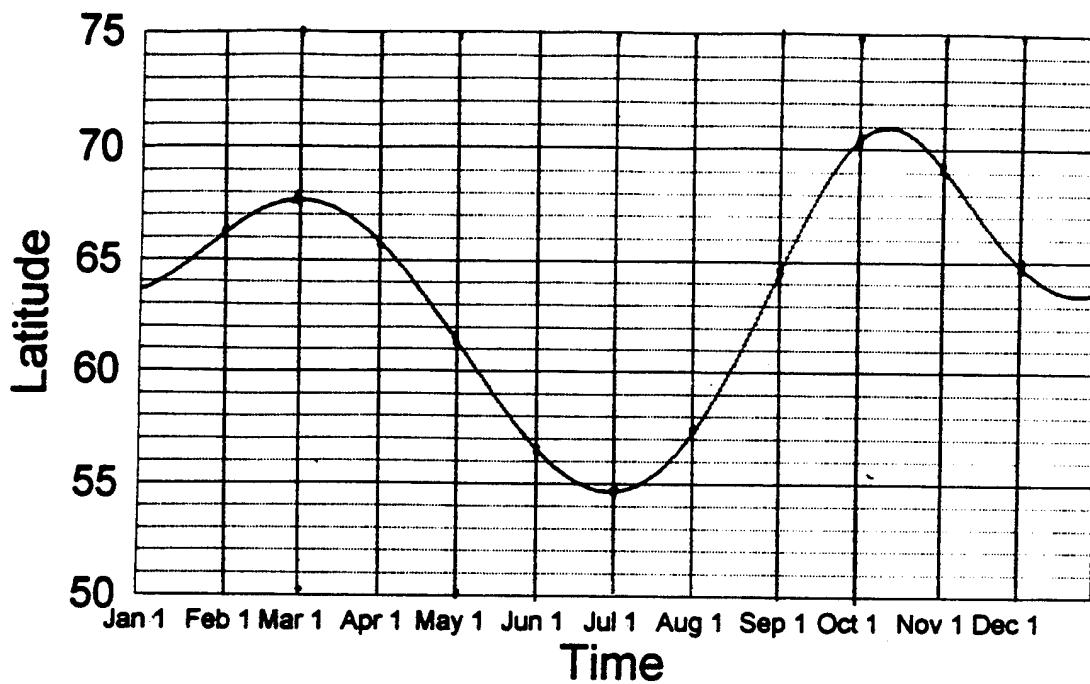
Figure 2: POAM II science sensors optical path arrangement.

# Atmospheric Extinction vs Wavelength at 18 km

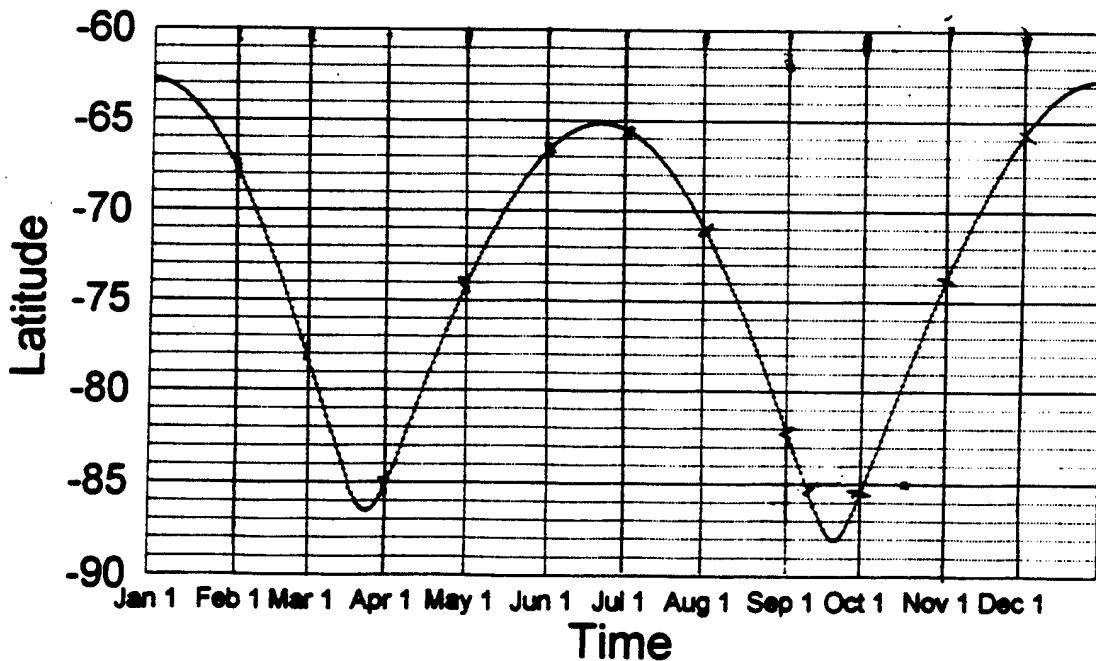
Wavelength (nm)	Width (nm)	Primary Purpose
353.0	5	Aerosols
442.0	2	$\text{NO}_2$ Off
448.3	2	$\text{NO}_2$ On
600.0	15	Ozone
760.8	2	$\text{O}_2$ On
780.0	15	$\text{O}_2$ Off
920.0	2	$\text{H}_2\text{O}$ Off
935.5	2	$\text{H}_2\text{O}$ On
1059.0	10	Aerosols

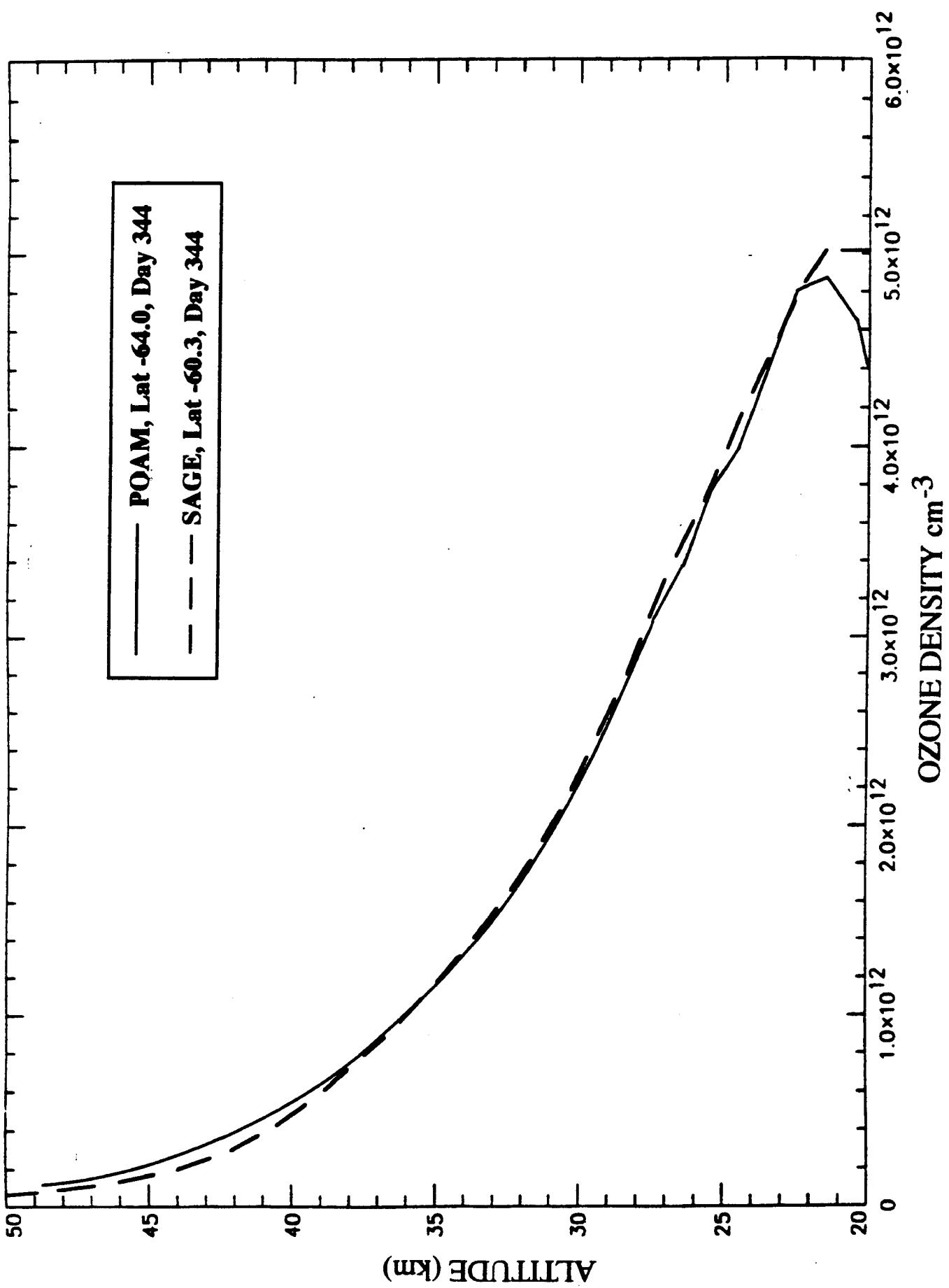


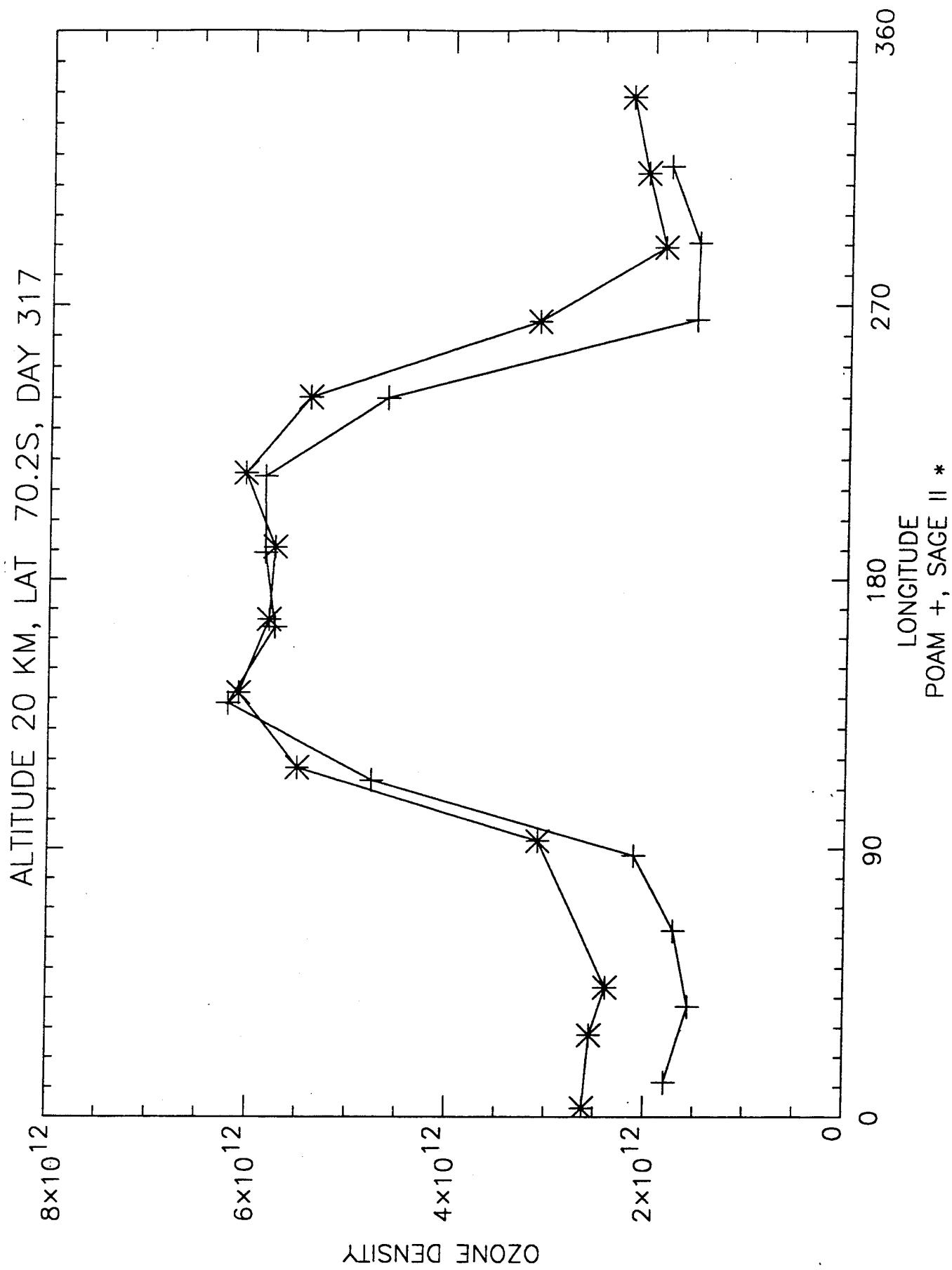
## **POAM II Sub-Tangent Latitude 1994 Sunrises**



## **POAM II Sub-Tangent Latitude 1994 Sunset**





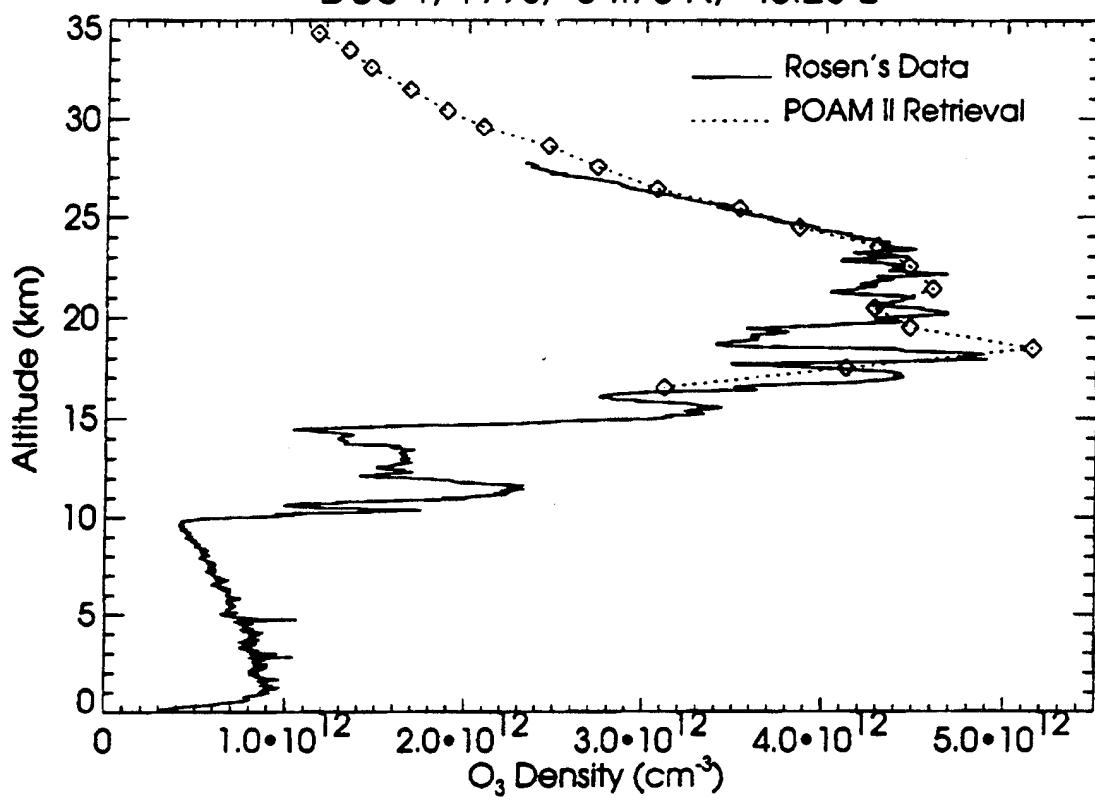


**POAM II Comparisons with University of Wyoming Balloon  
Measurements near Archangel, Russia (64.62° N 40.5° E)**

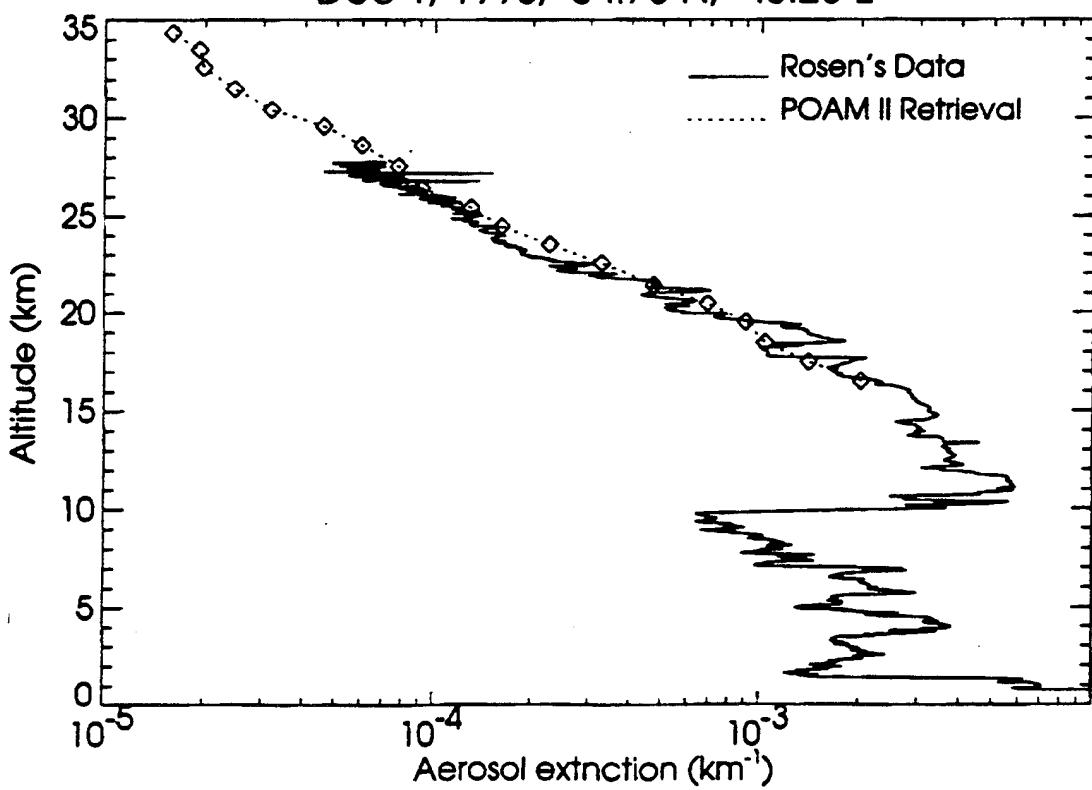
**Measurement Dates**

Date	Time (GMT)	20 km Tan. Latitude	20 km Tan. Longitude	Range (km)
Mon 29 Nov 93	1133	65.01	35.89	224
Wed 1 Dec 93	1054	64.78	45.28	229

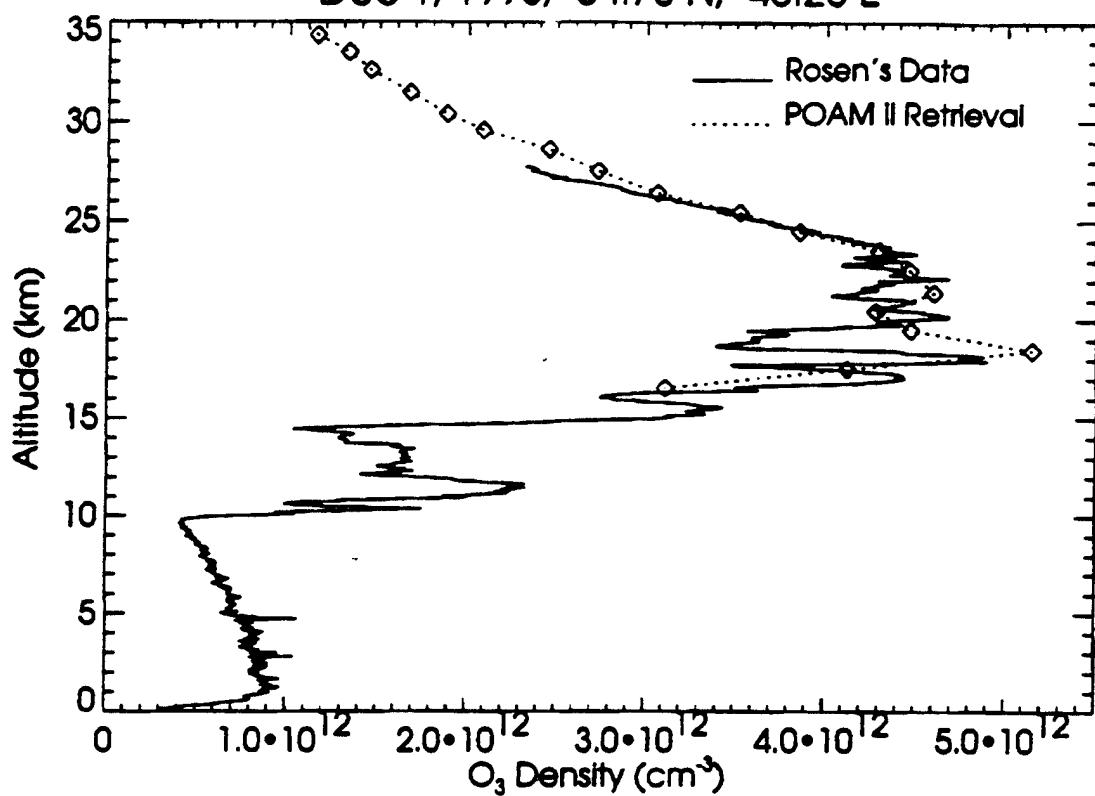
Dec 1, 1993, 64.78 N, 45.28 E



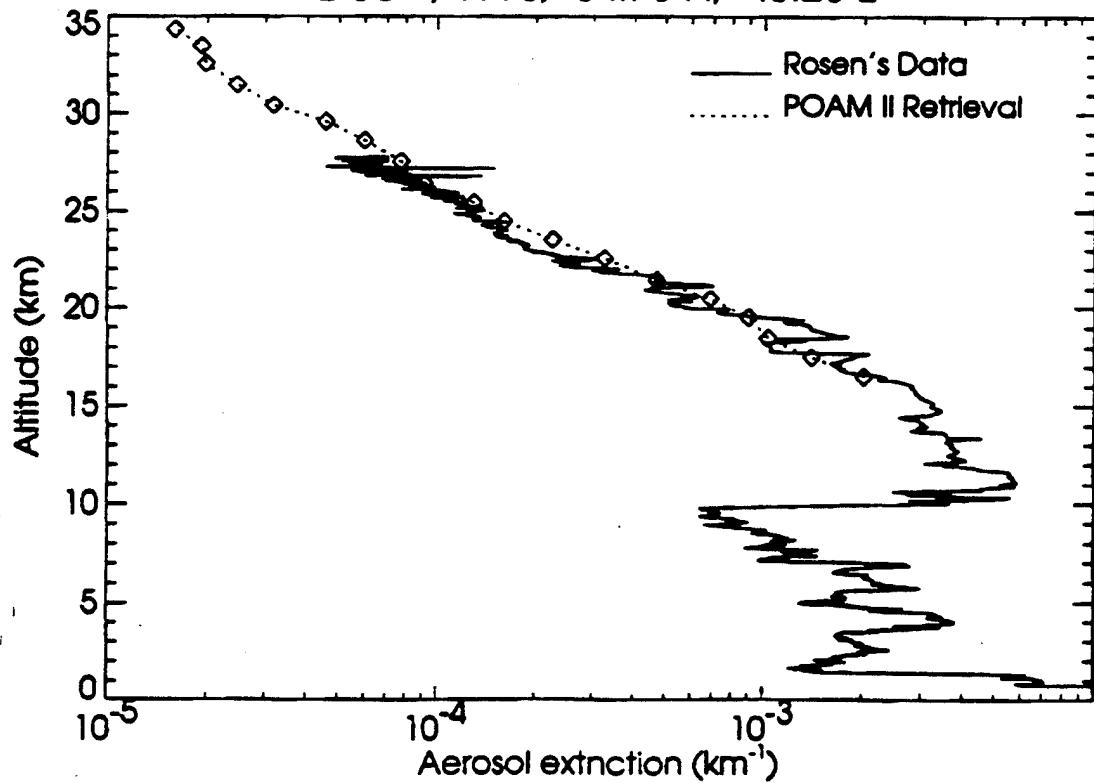
Dec 1, 1993, 64.78 N, 45.28 E



Dec 1, 1993, 64.78 N, 45.28 E



Dec 1, 1993, 64.78 N, 45.28 E

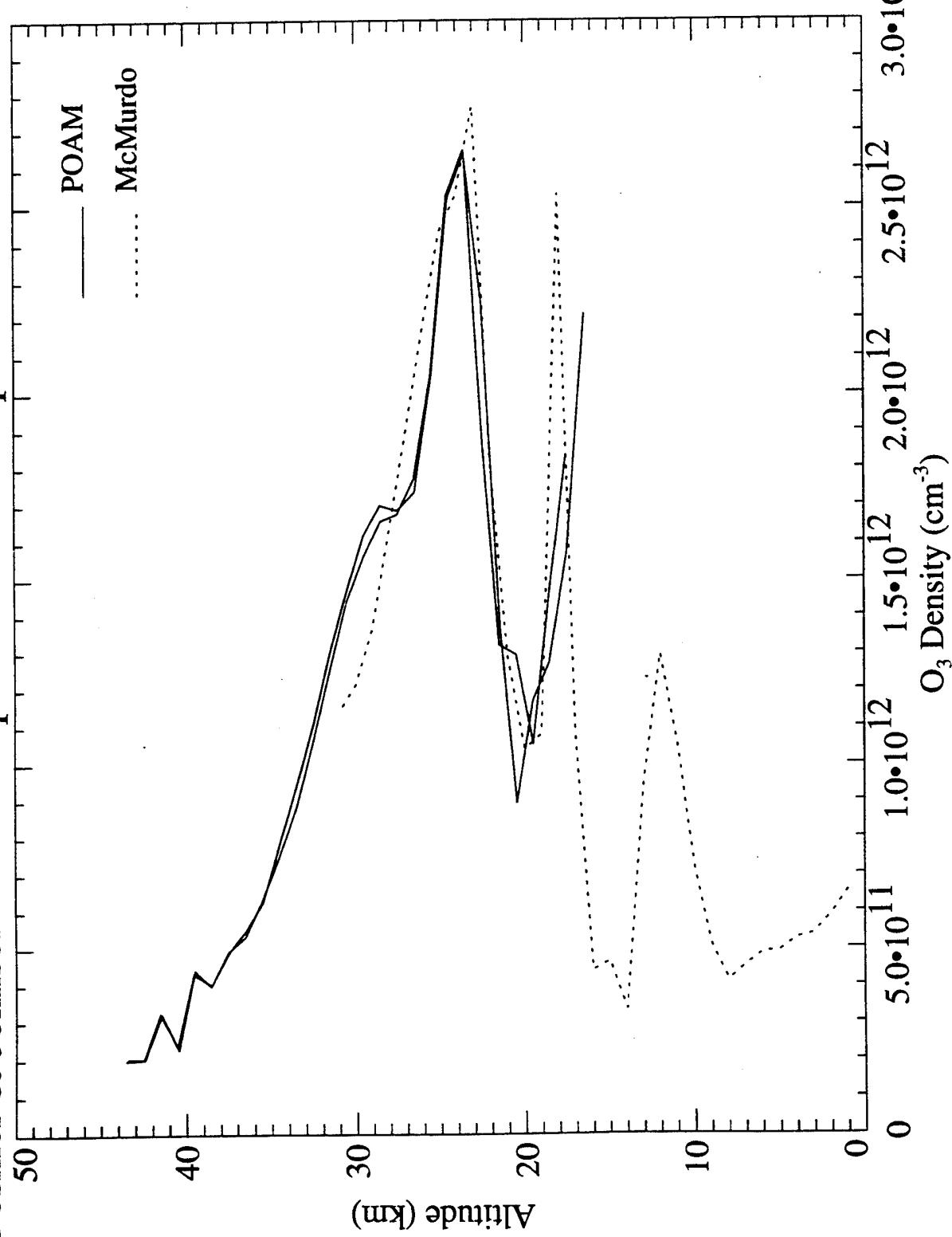


**POAM II Comparisons with University of Wyoming Balloon  
Measurements near McMurdo ( $78^{\circ}$  S  $167^{\circ}$  E)**

**Measurement Dates**

Date	POAM II Time (GMT)	20 km Tan. Latitude	20 km Tan. Longitude	Range (km)	Balloon Time (GMT)
16 Oct 93	1002	79.78	177.05	305	0100
	1143	79.75	151.67	404	15 Oct
23 Oct 93	1108	77.15	162.05	148	2200
28 Oct 93	1112	75.36	161.67	318	1100
30 Oct 93	1033	74.68	171.60	384	1000

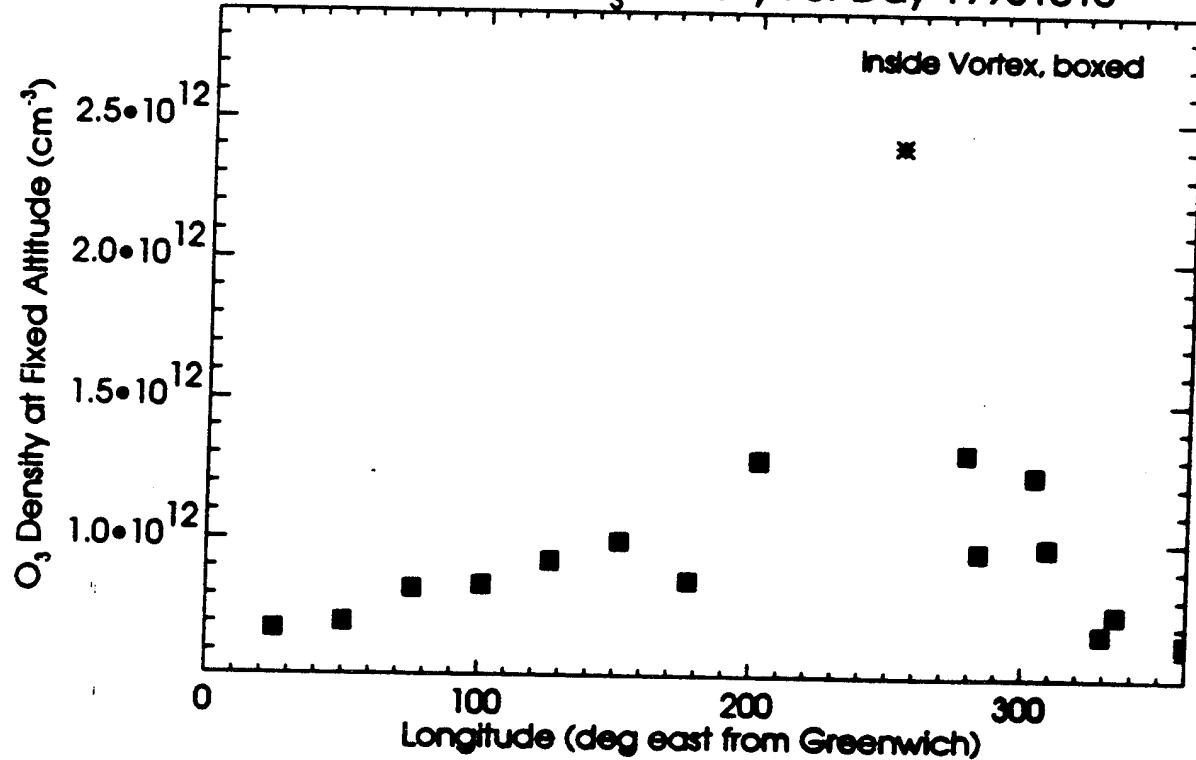
Deshler & Johnson McMurdo profile Oct 15 compared with POAM II Oct 16



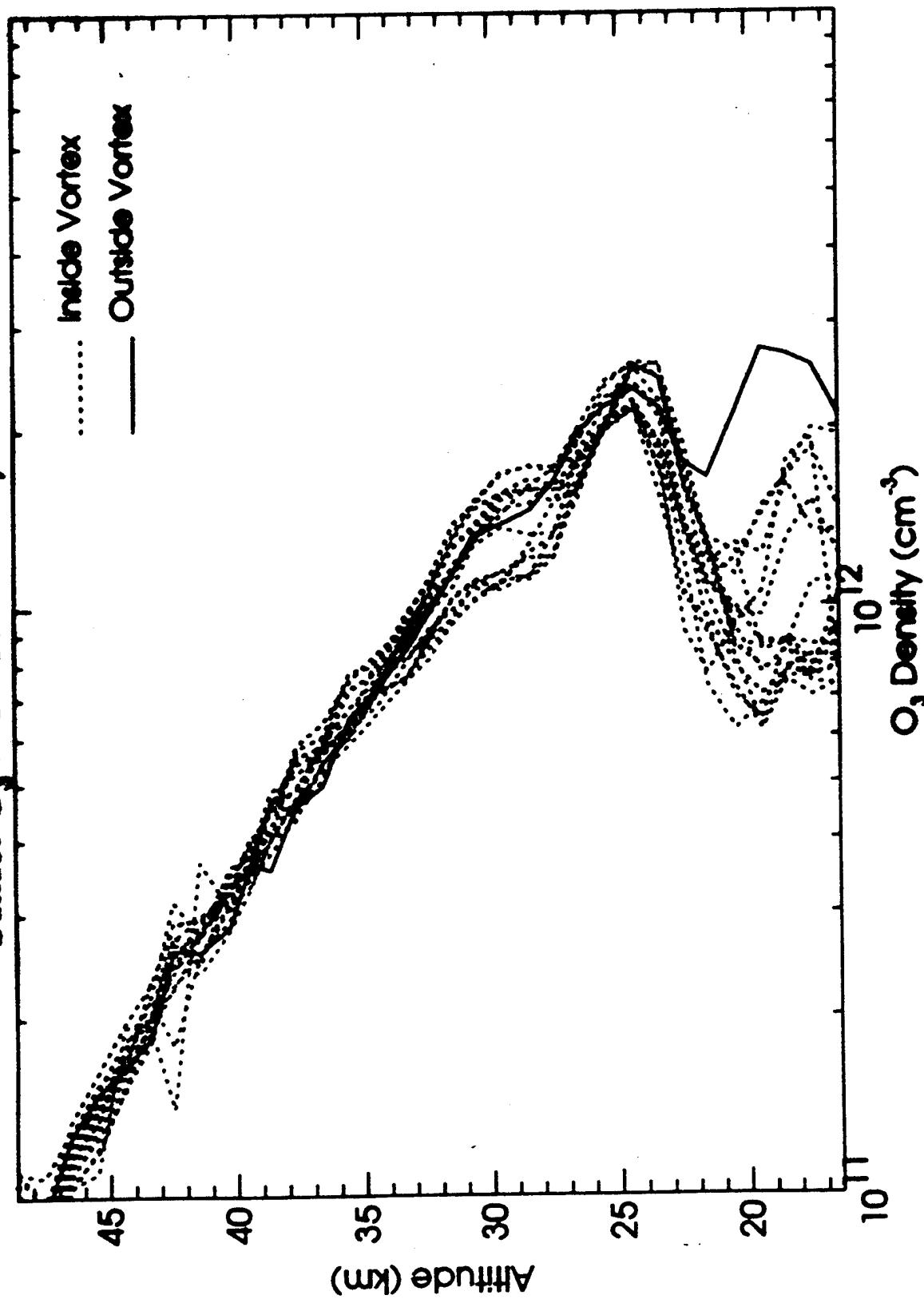
Polar Vortex & POAM Events: 931016



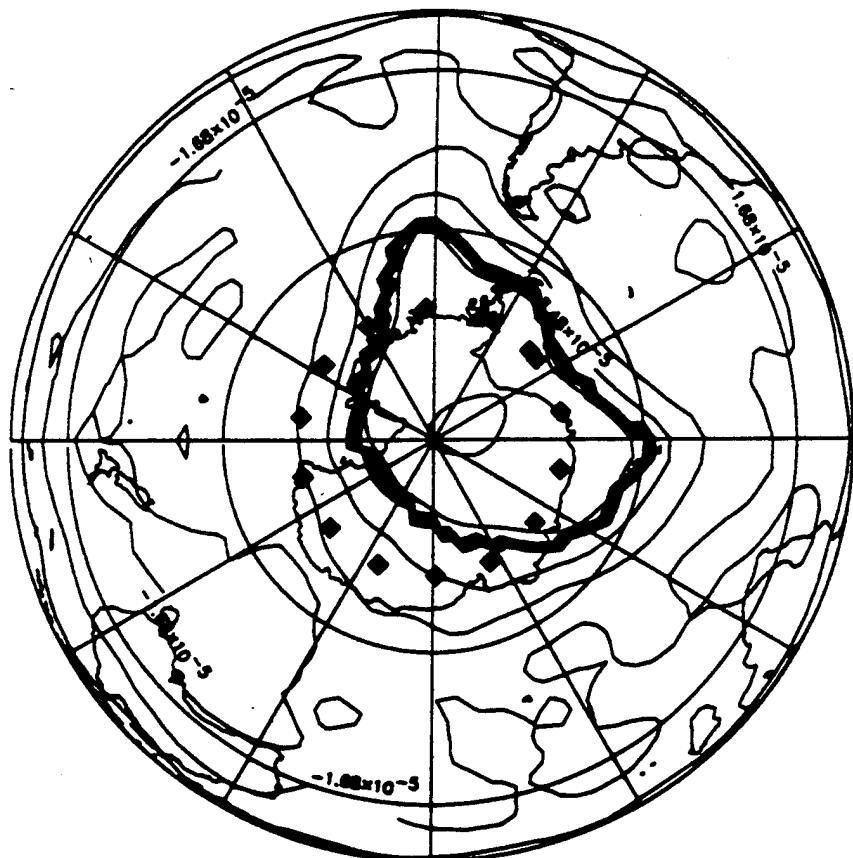
Sunset 20 km O<sub>3</sub> Density For Day 19931016



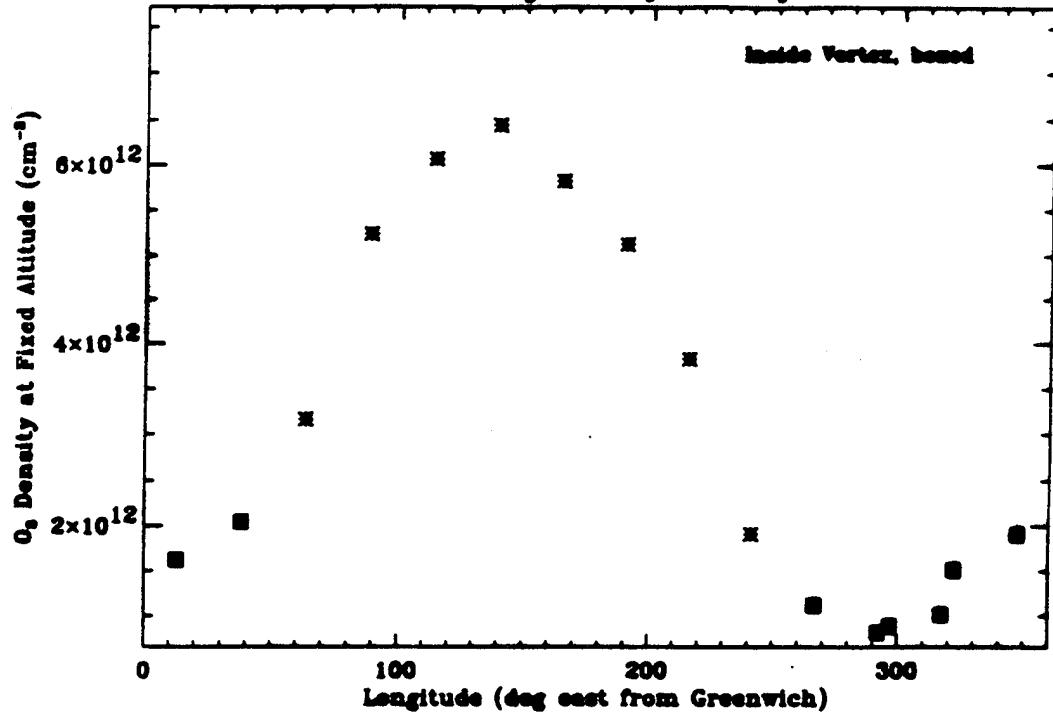
### Sunset O<sub>3</sub> Profiles For Day 19931016



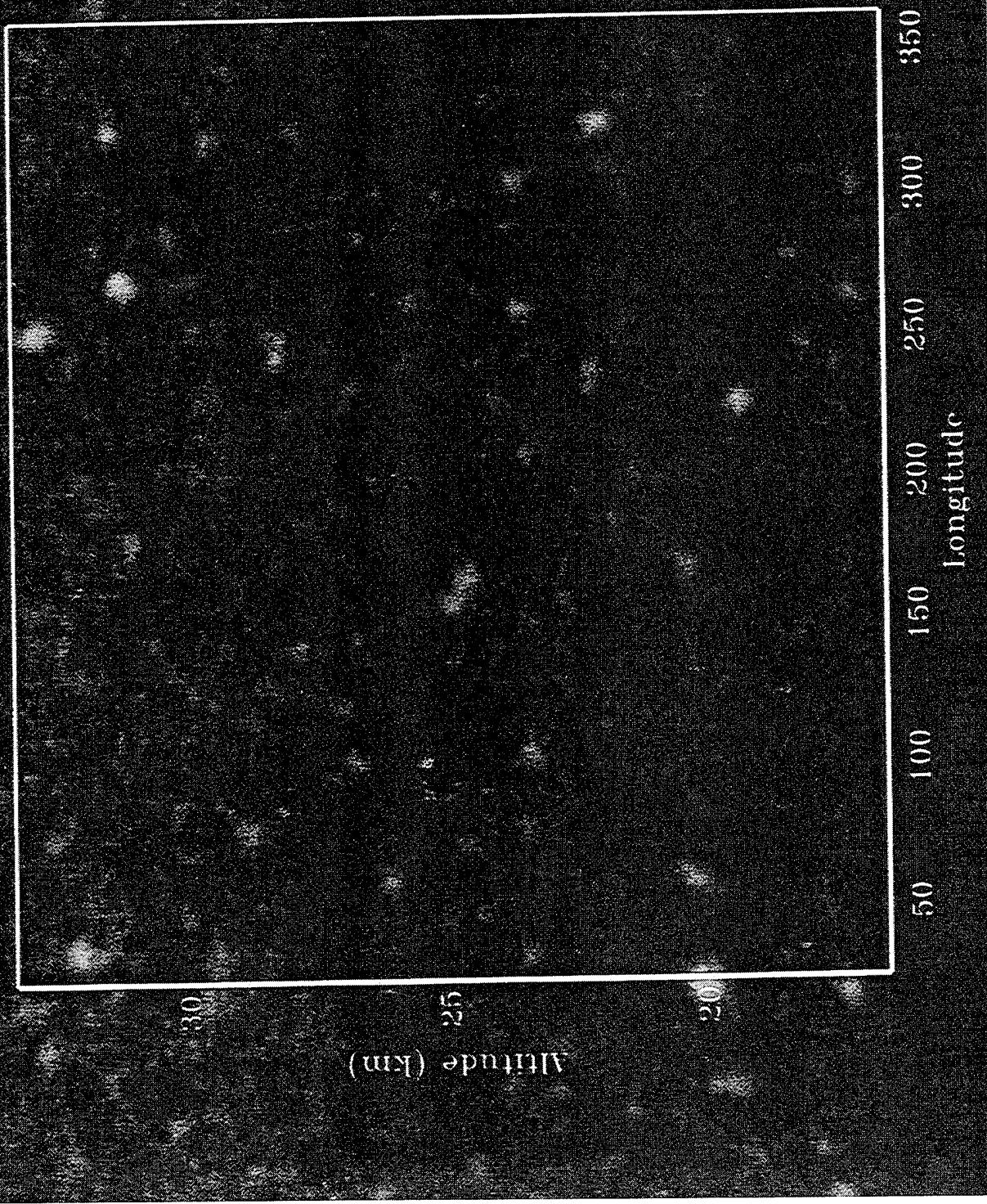
# Polar Vortex & POAM Events: 931108



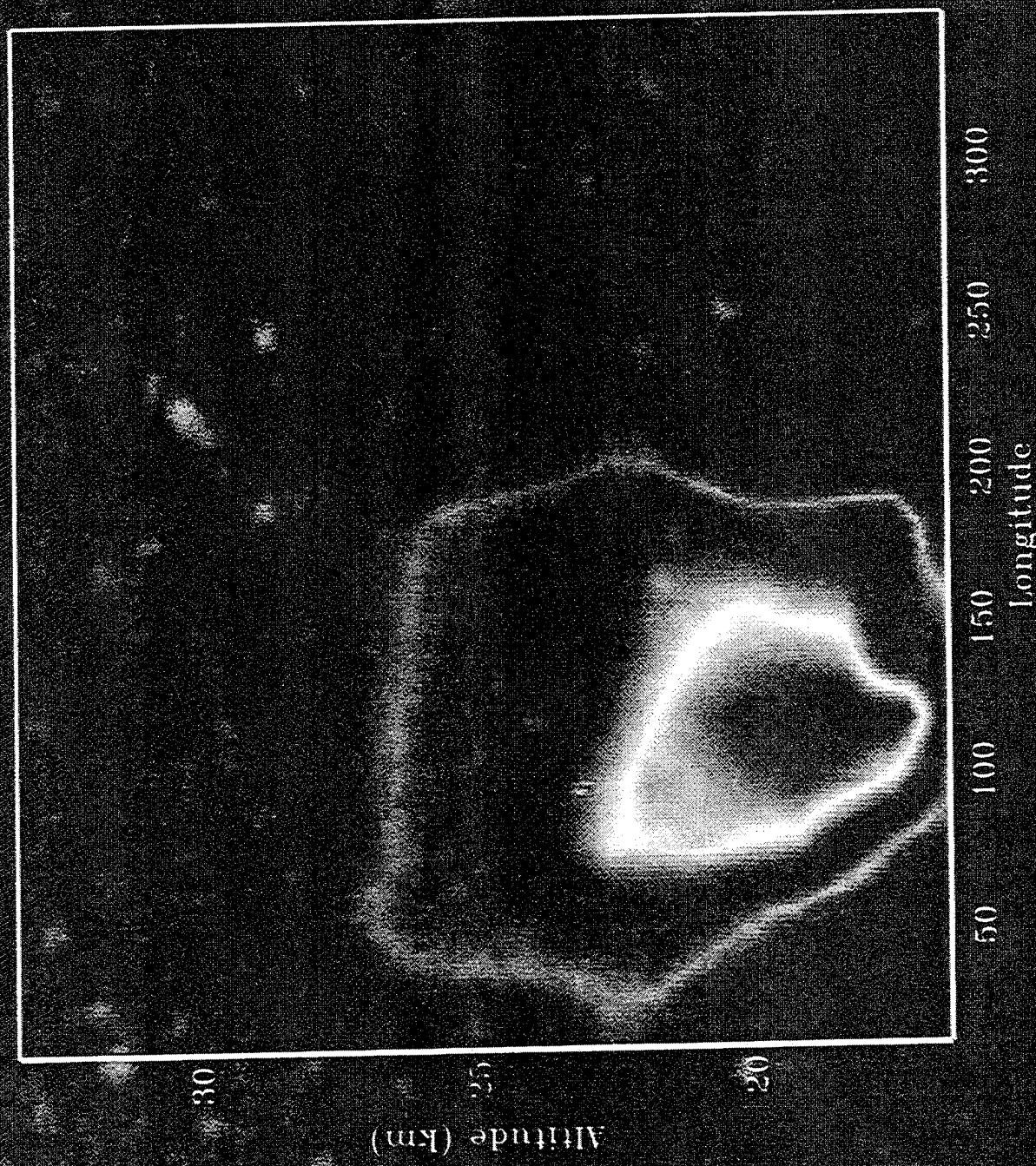
Sunset 20 km O<sub>3</sub> Density For Day 19931108



Ozone Concentration ( $\text{cm}^{-3}$ ) Variation Over 1 Day  
Southern Hemisphere For 10/16/93



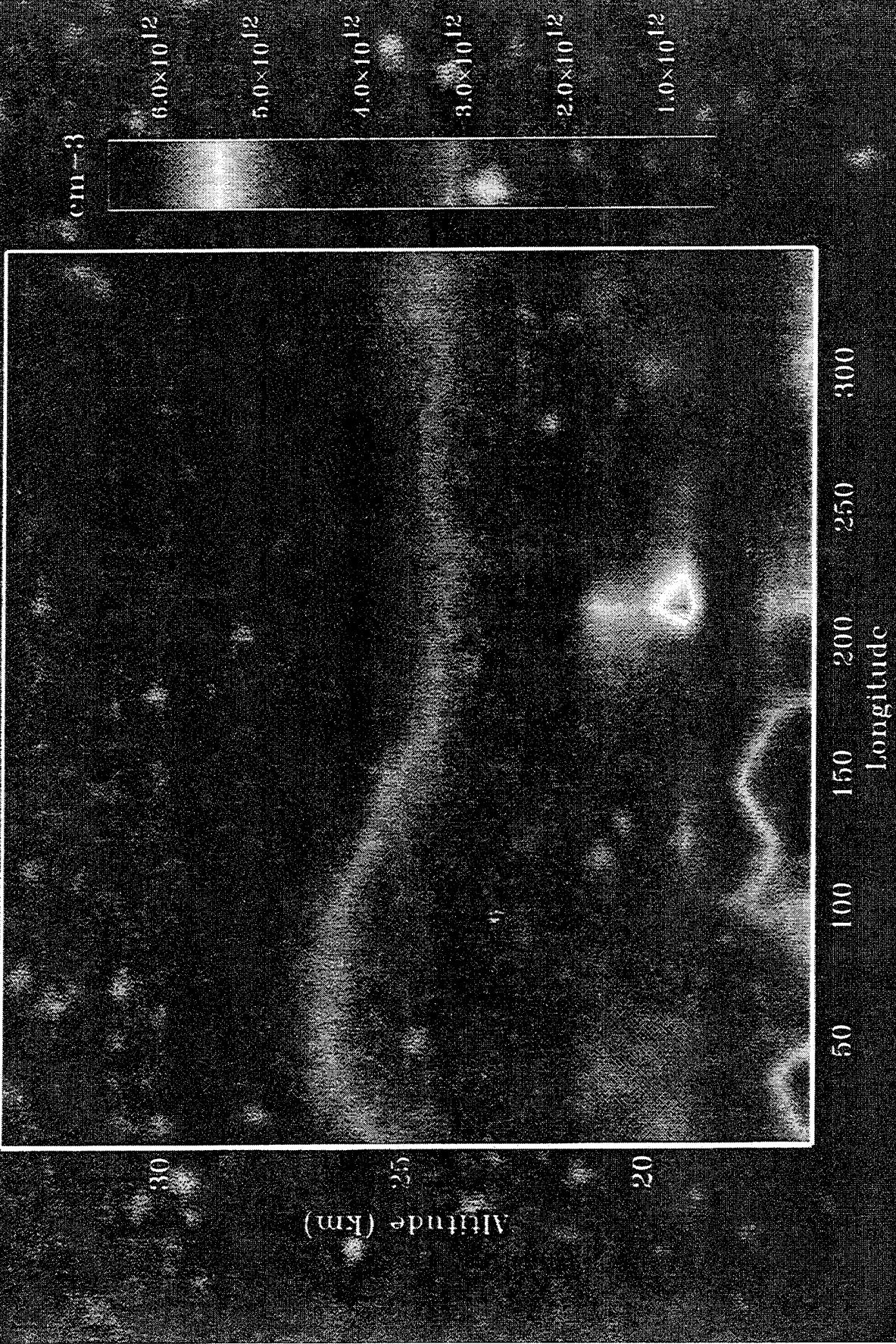
Ozone Concentration ( $\text{cm}^{-3}$ ) Variation Over 1 Day  
Southern Hemisphere For 11/08/93



Ozone Concentration ( $\text{cm}^{-3}$ ) Variation Over 1 Day  
Southern Hemisphere For 1/25/93



Ozone Concentration ( $\text{cm}^{-3}$ ) Variation Over 1 Day  
Southern Hemisphere for 12/20/93



Zonal Average Ozone Concentration ( $\text{cm}^{-3}$ )  
Southern Hemisphere Dissipation : 1993-1994



# Conclusions

- \* POAM II continues to operate well 8 months after launch.
- \* Validation of the Ozone retrievals is well under way.
- \* Validation of the other species has begun.

# **Large-Scale Retrieval of Atmospheric Parameter Profiles**

**Annual Review Conference on  
Atmospheric Transmission Models**

**June 8, 1994**

**L. Sparks, J.L. Fanselow, J. McComb,  
S. Nandi, J. Parker, and J.E. Patterson**

*Jet Propulsion Laboratory  
California Institute of Technology  
Pasadena, California 91109*

# Simulation / Data System

## Functional Schematic

RADIATIVE TRANSFER PROCESS

Observer

Sun

Scattering

Clouds

Pollution

Earth's Surface

Absorption

Wave number

Altitude

Abundance

## SEASCRAPE

### *Sequential Evaluation Algorithm for Simultaneous and Concurrent Retrieval of Atmospheric Parameter Estimates*

- **Sequential** parameter estimation that utilizes a Square Root Information Filter, allows the specification of *a priori* data and constraints, and provides a formal error analysis.
- **Simultaneous** retrieval of multiple atmospheric profiles and instrument parameters.
- **Concurrent** data analysis on a parallel processor.
- **Retrieval** algorithm integrates the forward model with the inversion algorithm (the forward model can stand alone as a simulation tool).

# ***Features of SEASCRAPE***

## ***Version 1.0***

- Nadir sounding.
- Retrieval of temperature, pressure, and constituent profiles.
- Simultaneous processing of multiple spectra.
- One dimensional model (spherical symmetry).
- Homogeneous layers with arbitrary spacing.
- Refraction (discontinuous refractive index).
- Parameters defined at zone boundaries, where a zone consists of one or more layers.
- Constraints, and *a priori*:
  - A. Hydrostatic equilibrium.
  - B. Parameter ranges.

## *Features of SEASCRAPE (cont.)*

### *Version 1.0*

- Absorption/emission spectra (modeled on a line-by-line basis).
- Continuum absorption: H<sub>2</sub>O, CO<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>.
- Absorption cross sections for species where individual lines cannot be modeled.
- Modeling and retrieval of surface brightness temperature.
- Formal, quantitative error analysis.
- SEA\_Front, a menu-driven front-end for operating SEASCRAPE.
- Public domain software with anonymous FTP access.

## ***Features of SEASCRAPE (cont.)***

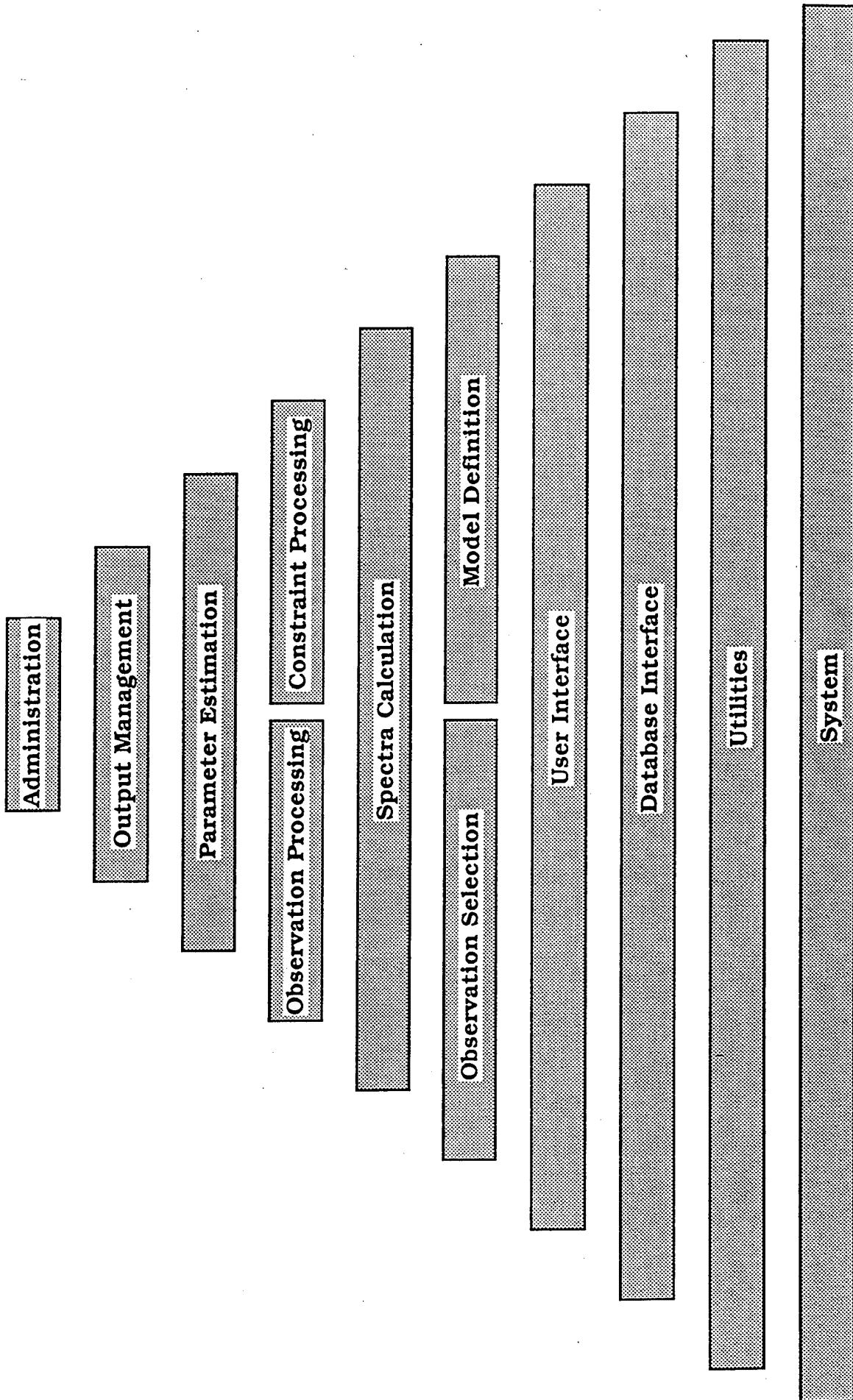
### ***Version 2.0 and beyond***

- Implementation in a parallel processing environment.
- Limb and nadir sounding.
- Ground emission and reflection.
- Multi-dimensional atmospheric model.
- Inhomogeneous cells:
  - A. Improved ray-tracing.
  - B. Improved integration of the equation of radiative transfer.
  - C. Improved hydrostatic equilibrium.
- Clouds, aerosols, and scattering, possibility incorporating existing electromagnetic scattering codes.
- Retrieval of instrumental parameters.

## ***Applications***

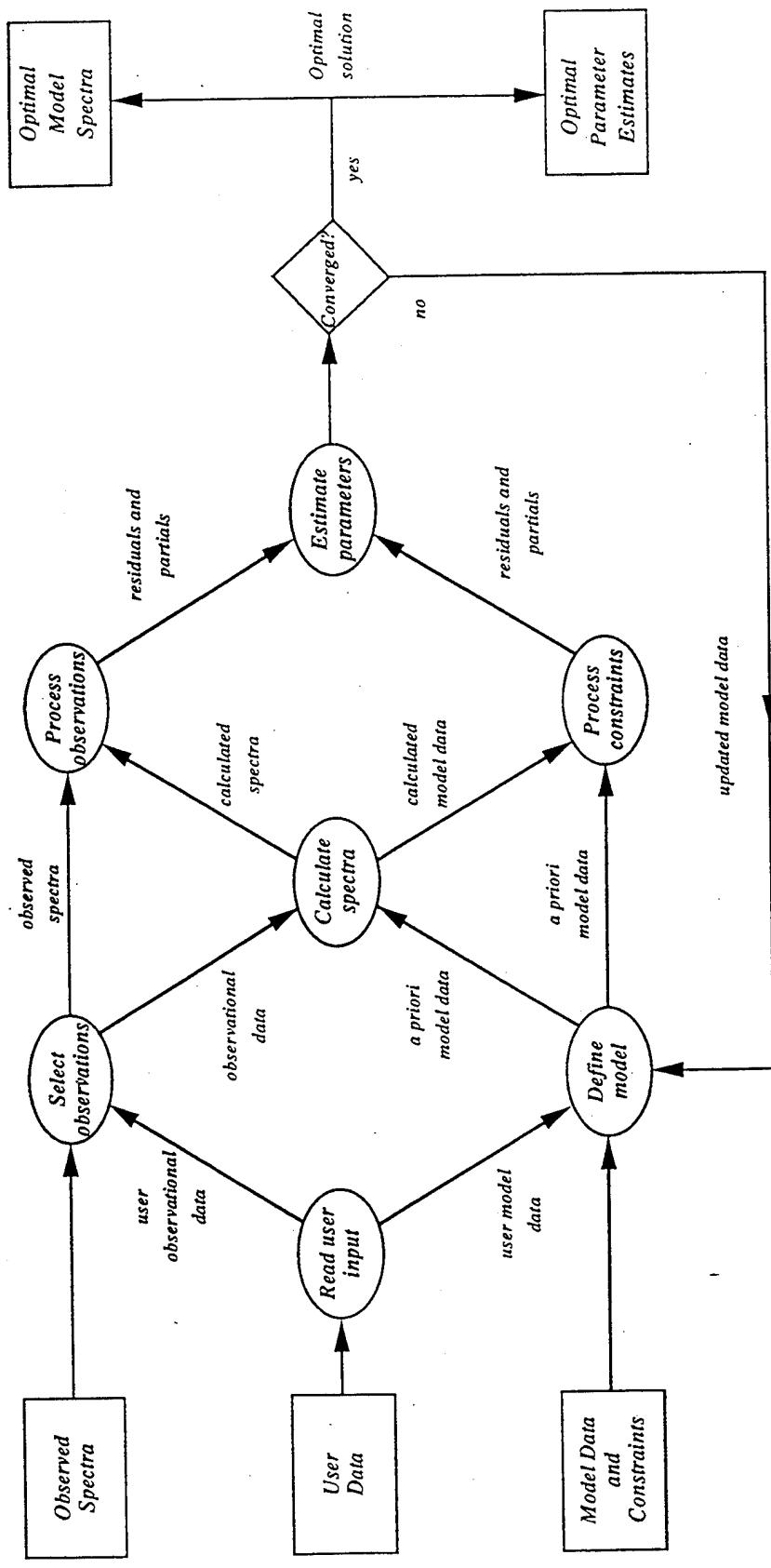
- Airborne Emission Spectrometer (AES) - nadir sounding, emission spectra
- Deep Space Network (DSN) - uplooking retrieval of water vapor profiles, emission spectra
- ATMOS Fourier Transform Spectrometer (FTS) for the ATLAS Shuttle payload - limb sounding, transmission spectra
- Spectroscopic community- simulation studies
- Tropospheric Emission Spectrometer (TES) for Eos - nadir and limb sounding, emission spectra

# **Structure of SEASCRAPE**



# SEASCRAPE

## Data Flow



## *Forward Model*

Radiation reaching the instrument is a function of the radiation emitted, scattered and absorbed by the atmosphere as well as the radiation emitted and reflected by the background.

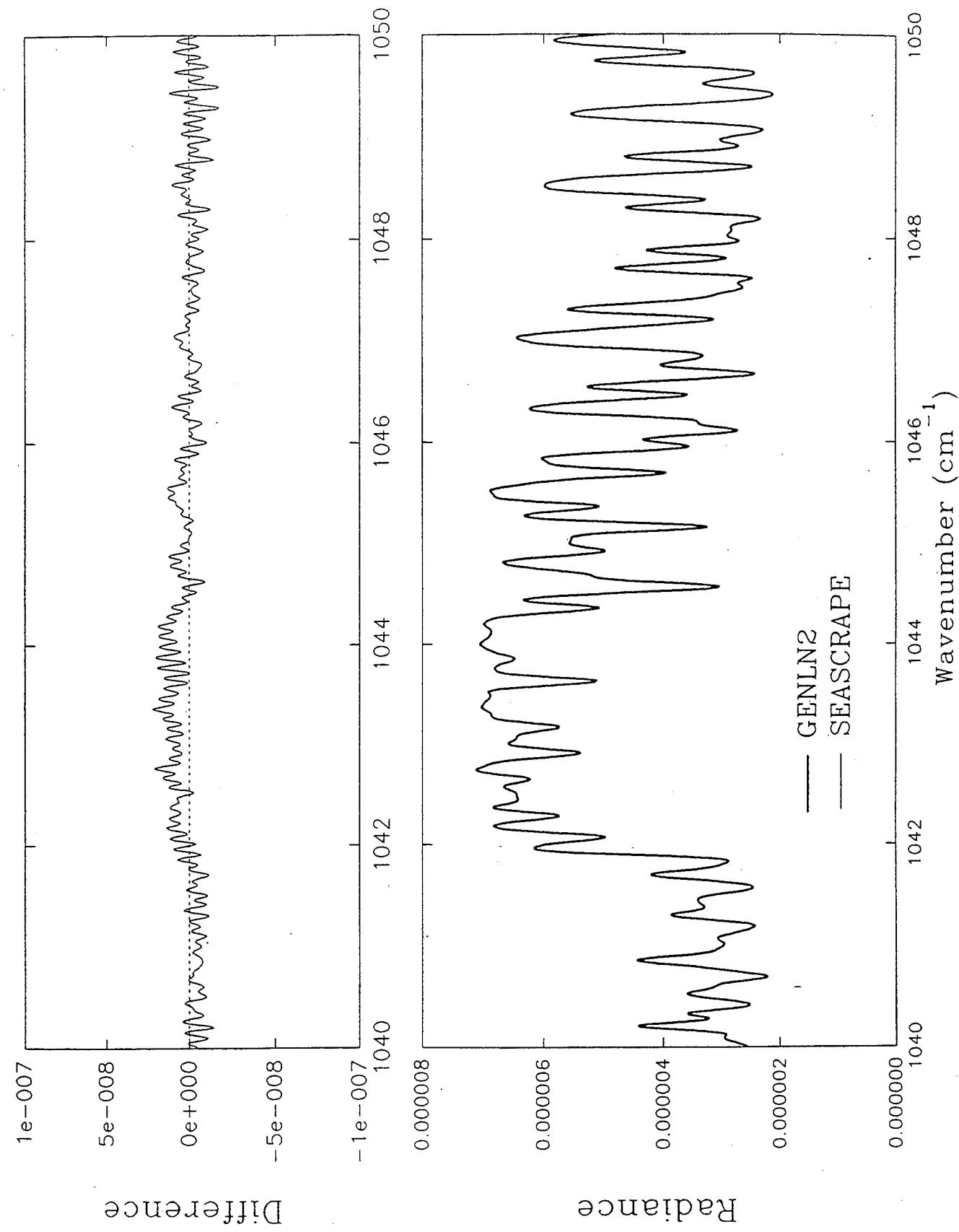
Equation of radiative transfer:

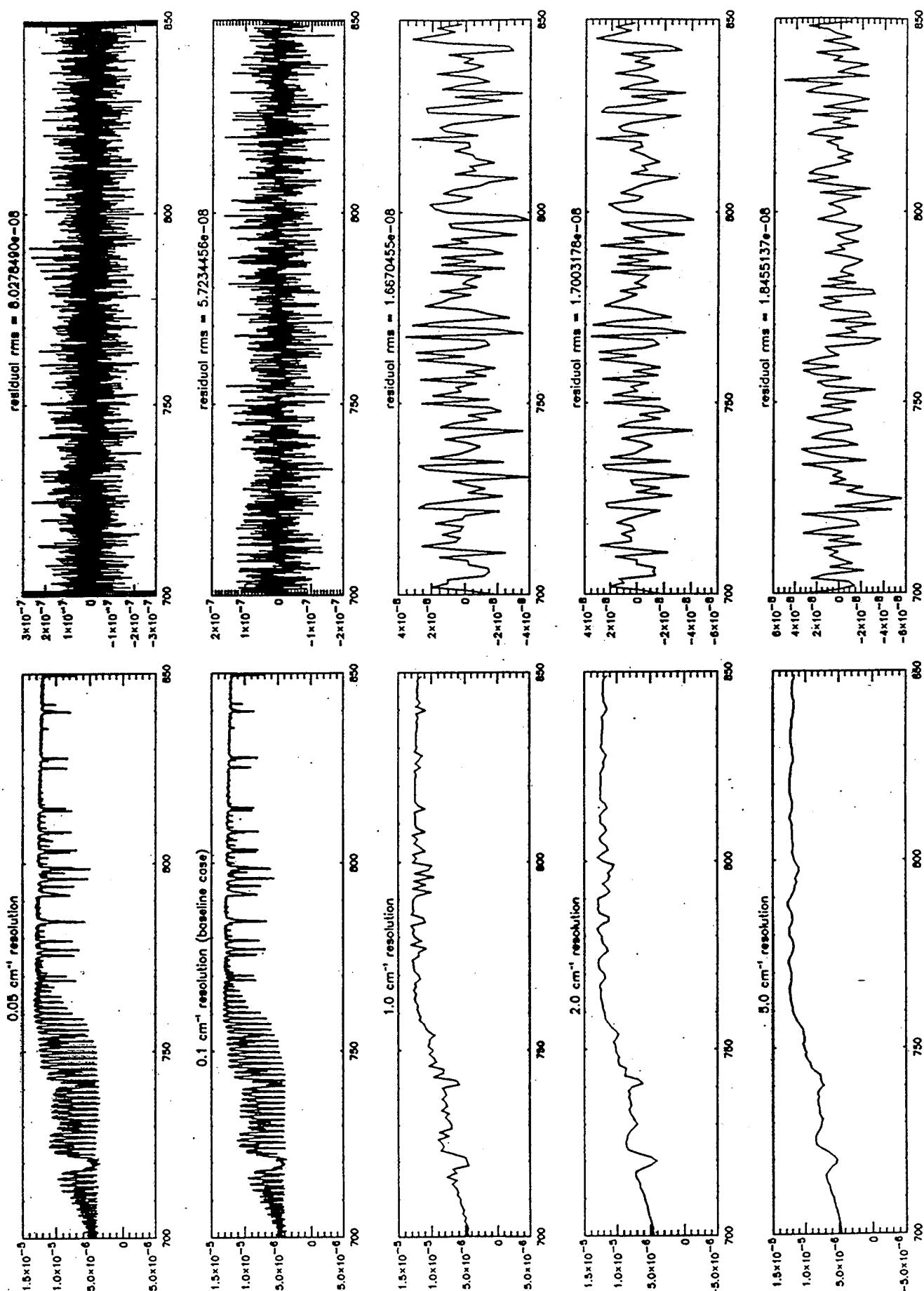
$$\frac{\partial J(v,s)}{\partial s} = -\kappa(v,s)[J(v,s) - B(v,s)]$$

where

- |               |                           |
|---------------|---------------------------|
| $J(v,s)$      | ≡ radiance;               |
| $\kappa(v,s)$ | ≡ extinction coefficient; |
| $B(v,s)$      | ≡ thermal emission;       |
| $v$           | ≡ frequency;              |
| $s$           | ≡ path length;            |

GENLN2 vs. SEASCRAPE - Case 2aa





## Parameter Estimation

Processing observations:

$$\bar{J}_\nu = J_\nu + \sum_{n=0}^N \frac{\partial J_\nu}{\partial \Lambda_n} \Delta \Lambda_n + \varepsilon_\nu$$

where  $\bar{J}_\nu$   $\equiv$  observed radiance;  
 $J_\nu$   $\equiv$  modeled radiance;  
 $\Delta \Lambda_n$   $\equiv$  parameters to be estimated;  
 $\varepsilon_\nu$   $\equiv$  error;

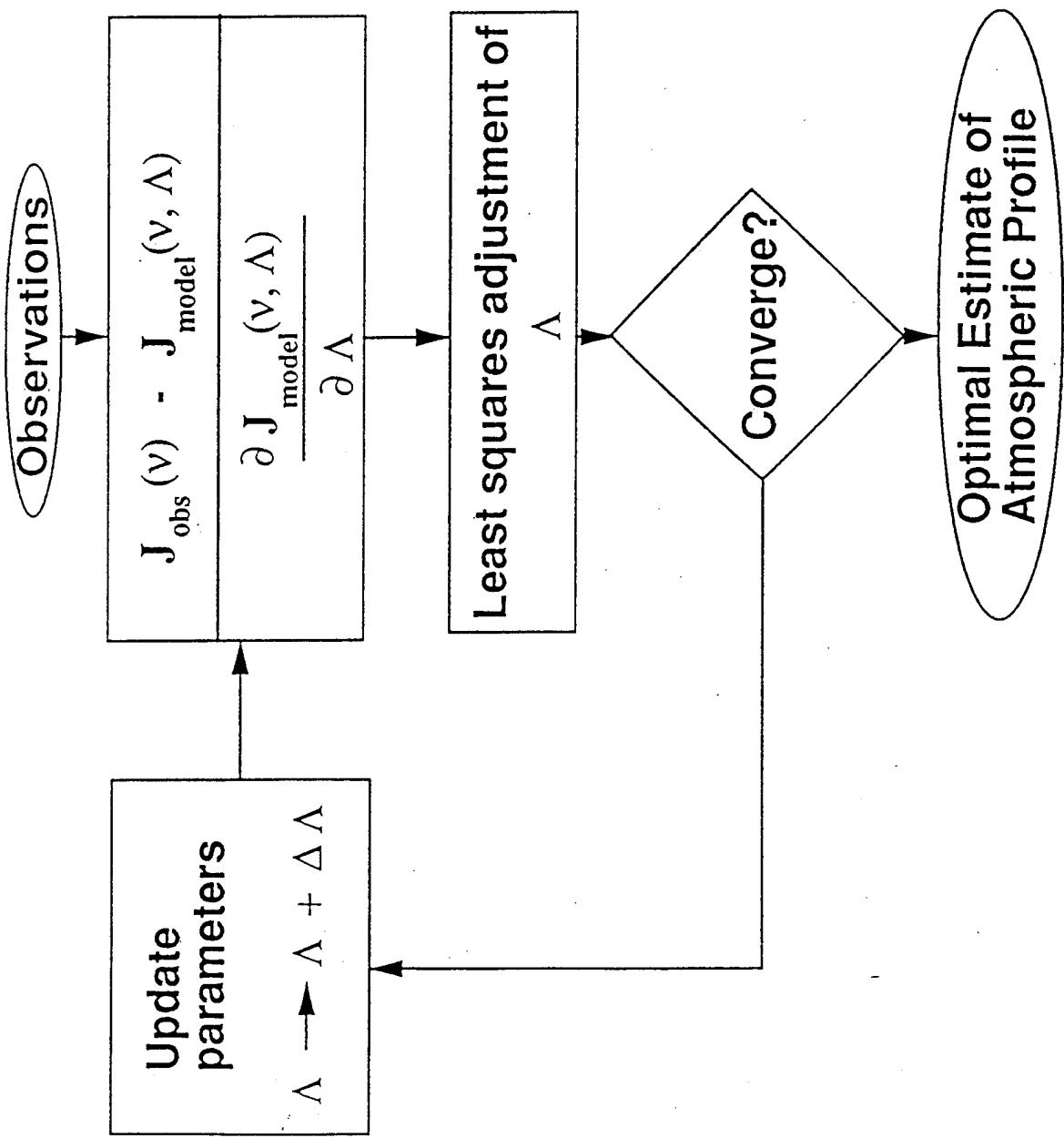
Processing constraints:

$$\bar{f} = f + \sum_{n=0}^N \frac{\partial f}{\partial \Lambda_n} \Delta \Lambda_n + \varepsilon$$

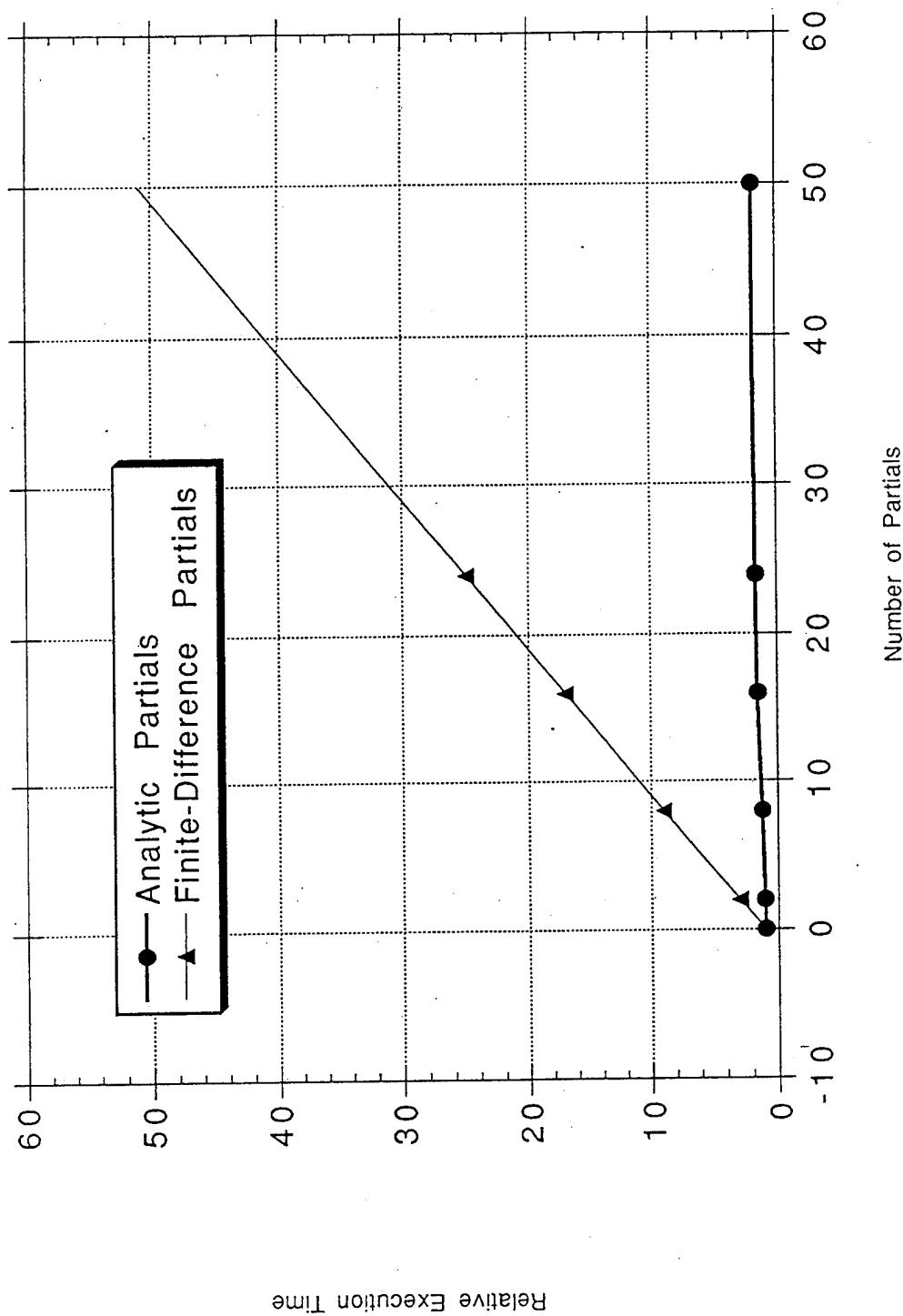
where  $\bar{f}$   $\equiv$  imposed value of constraint;  
 $f$   $\equiv$  estimated value of constraint;  
 $\Delta \Lambda_n$   $\equiv$  error.

Solve for  $\Delta \Lambda_n$ .

# Least Squares Process



Execution Time vs. Number of Partialials



Relative Execution Time

## Error Analysis

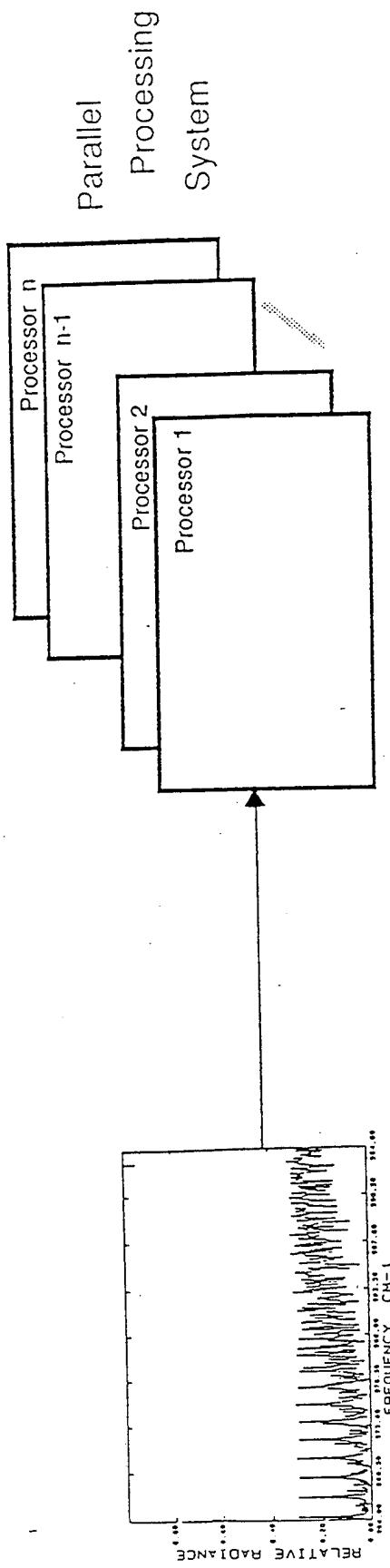
In addition to retrieving parameter profiles, the estimation algorithm provides a systematic, quantitative error analysis:

$$\left. \begin{array}{l} \text{Observational error (i.e., noise)} \\ \text{A priori model error} \end{array} \right\} \Rightarrow \text{Parameter error}$$

The output parameter error covariance matrix describes quantitatively:

- the uncertainty of the retrieved parameters;
- correlations between the errors in the retrieved parameters;
- the optimal parameterization of the observational model.

## Parallel Implementation of SEASCAPE



In the parallel decomposition of SEASCAPE, each processor

- receives a frequency window of the observed spectrum
  - has resident in memory its section of the line list data base
  - forms its own SRI/F matrix for the estimated parameters which is then combined with the SRI/F matrices from the other processors
- Processor attributes:
- MIMD (each processor must be independent to avoid serious load imbalance)
  - high performance (10 - 30 MFLOPS)
  - large DRAM (16-64 megabytes)

Oder

---

A GENERAL INVERSION PACKAGE FOR ADVANCED  
RETRIEVAL OF ATMOSPHERIC SPECIES FROM  
HIGH SPECTRAL RESOLUTION MEASUREMENTS

J.L. MONCET  
W.O. GALLERY

ATMOSPHERIC AND ENVIRONMENTAL RESEARCH, INC.

Annual Review Conference on Transmission Models  
Phillips Laboratory, Hanscom AFB, MA  
June 7-8, 1994

## Introduction

---

- Goal: to develop a generic research grade inversion code
  - Simultaneous retrieval of atmospheric temperature and/or atmospheric species concentration (water vapor and trace species)
  - Applied to high spectral resolution radiance measurements.
- Main Features:
  - Based on non-linear least-squares inversion technique
  - Radiative transfer (forward model)
    - Currently uses optical depth calculation from FASCODE plus internal layer looping interface for user-supplied forward model: exact (line-by-line) or approximate (e.g. MODTRAN)
  - Applicable to any viewing geometry: upward/downward/limb and can accommodate any instrument type from microwave to IR sounder (satellite or balloon borne, or ground based)

## Introduction (continued)

---

- Some Requirements:
  - Computationally fast
  - Flexible user input (can easily select retrievable species, atmospheric layering, viewing geometry, instrument characteristics,...)
  - Allows the retrieval of non-atmospheric parameters (spectroscopic parameters, calibration parameters, tangent height for limb case ...)
  
- Applications
  - Actual data analysis and exploration fo the retrieval capability of particular instrument designs (e.g. DBIS, SCRIBE, CIRRIS, MSSX)
  - Retrieval simulations for sensor design trade studies (MOES, AIRS, ITS)
  - Benchmarking fast forward model parameterizations or non-optimal retrieval approaches (e.g. onion peeling) used in operational applications

## Comparison with Current Operational Retrieval Algorithms

---

- A number of specialized non-linear inversion codes are already available or being developed for various applications (e.g. AIRS program, UARS)
  - These codes use fast parameterizations of the atmospheric transmission for each individual molecular species (e.g. McMillin and Fleming, 1976, Eyre and Woolf)
  - Issues:
    - Process of parameterizing the forward model may be expensive (requires multiple runs of reference line-by-line model and validation)
    - Algorithm bound to a specific instrument design and atmospheric representation (vertical layering,...etc.)
    - Parameterization of the forward model not error free and the impact on the retrieval product is generally not known
- => Fast parameterization is impractical at an exploratory stage
- Difficult/expensive to vary instrument characteristics and to revise spectroscopic parameters and atmospheric representation
  - Answer:
    - Need to sacrifice actual execution time for enhanced flexibility and versatility

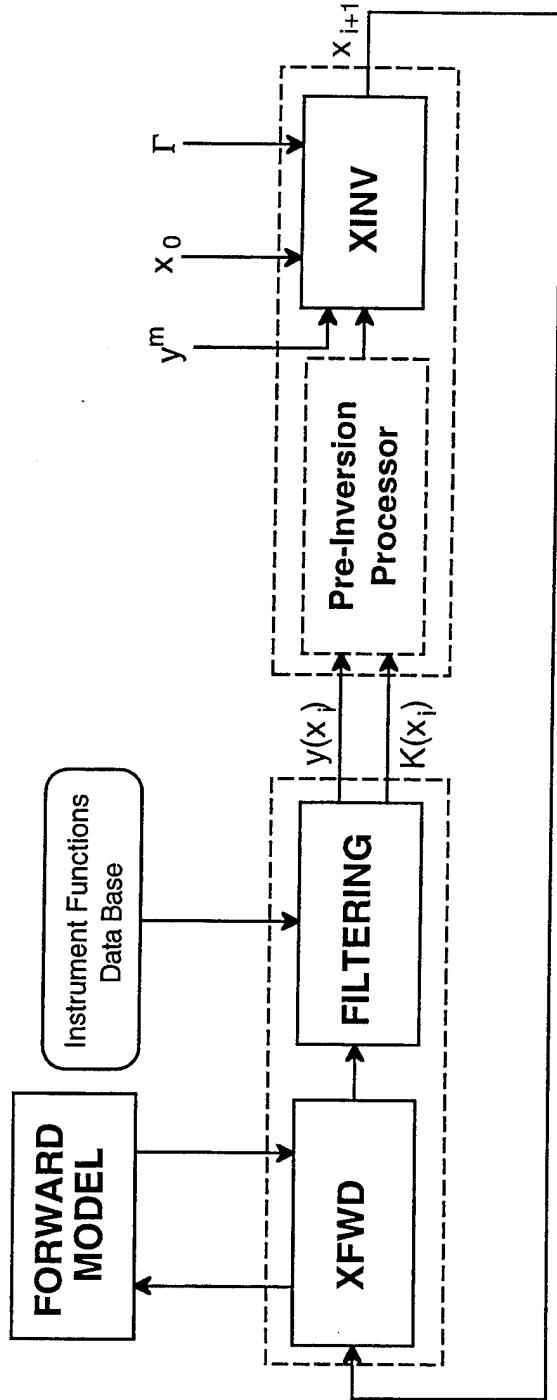
## General Code Description

---

- 4 separate modules:
  - Radiative transfer (XFWS)
  - Filtering
  - Pre-inversion processor
  - Inversion (XINV)
- Can be run interactively and independently or run together controlled by script
- Atmospheric layering implicit in the definition of the first-guess
- Unique input control file for all 4 modules used to:
  - Select viewing geometry (by specifying instrument altitude and viewing angle(s))
  - Select instrument function from preset filter bank
  - Select any of the 35 standard HITRAN molecular species to be retrieved simultaneously over specified altitude range (extended in the future to heavy molecules)
- XFWD uses atmospheric optical depths generated by an external forward model (runs currently with FASCODE routine HIRAC1). Radiative transfer is done internally by XFWD
- Interface for external forward model (e.g. MODTRAN)

Oder

## Block Diagram of Retrieval Algorithm



$x_0$  = background (first-guess) atmospheric profile

$x_i$  = estimated atmospheric profile at iteration  $i$

$y(x)$  = calculated radiances

$y^m$  = radiance measurements

$K(x_i)$  = Jacobian or sensitivity matrix

$\Gamma$  = matrix of "damping" coefficients

## Optimal Retrieval Approach (see Rodgers, 1976 and Eyre, 1989)

---

- Simultaneous retrieval of all species concentration at all atmospheric levels from available measurements
- Non-linear least-squares method based on Newton iteration procedure
- Optimal solution  $\hat{x}$  is such that the following cost function is minimized

$$J(x) = (y^m - y(x))^t w (y^m - y(x)) + (x - x_o)^t \Gamma (x - x_o)$$

- Solved by linearizing forward model around current guess at each iteration step:  
 $\delta y = K \delta x$  ;  $K$  is the Jacobian - calculated in XFWD

- The optimal solution is

$$x_i = x_{i-1} + H^{-1} [K^t w (y^m - y(x_{i-1})) + \Gamma (x_0 - x_{i-1})]$$

where

$$H = (K^t w K + \Gamma)$$

- $\Gamma$  can be manually tuned or evaluated from background error statistics when available (maximum probability solution (see Rodgers, 1976)

Oer

## Radiative Transfer Algorithm

- Start with layer furthest away from the observer (layer 1 in upward looking case)

### LAYER 1

1a) calculate  $\varepsilon_1$  and  $\frac{\partial \varepsilon_1}{\partial \tau_1}$

$$1b) \text{ calculate } \frac{\partial y}{\partial q_{1,m}} = \frac{\partial \varepsilon_1}{\partial \tau_1} \times \frac{\partial \tau_1}{\partial u_{1,m}} \times \frac{\partial u_{1,m}}{\partial q_{1,m}}$$

for m = 1,...M (number of constituents)

1c) update  $\sigma_1 = \varepsilon_1$

### LAYER 2

2a) calculate  $\varepsilon_2$  and  $\frac{\partial \varepsilon_2}{\partial \tau_2}$

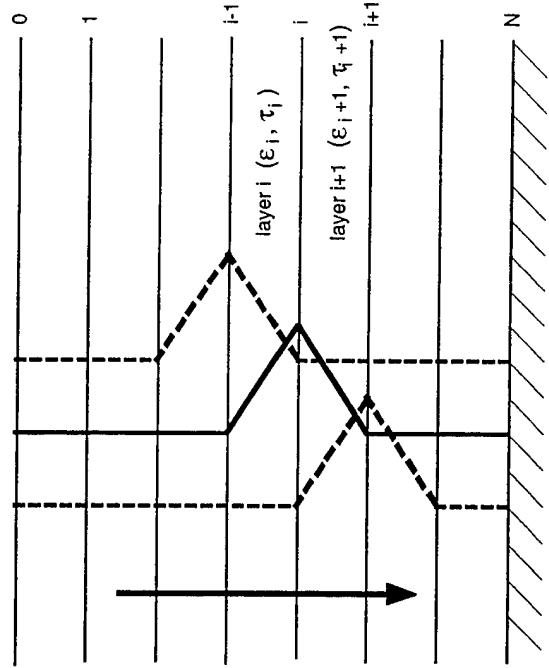
$$2b) \text{ calculate } \frac{\partial y}{\partial q_{1,m}} = \frac{\partial y}{\partial q_{1,m}} + \left( \frac{\partial \varepsilon_2}{\partial \tau_2} - \sigma_1 \right) \times \frac{\partial \tau_2}{\partial u_{2,m}} \times \frac{\partial u_{2,m}}{\partial q_{1,m}}$$

$$\text{and } \frac{\partial y}{\partial q_{2,m}} = \left( \frac{\partial \varepsilon_2}{\partial \tau_2} - \sigma_1 \right) \times \frac{\partial \tau_2}{\partial u_{2,m}} \times \frac{\partial u_{2,m}}{\partial q_{2,m}}$$

for m=1,...M (number of constituents)

2c) update  $\sigma_2 = \sigma_1 + \varepsilon_2$

REPEAT 2a,b,c FOR LAYER 3 AND SUBSEQUENT LAYERS



$\tau_i$  = layer optical depth

$\varepsilon_i = \varepsilon(\tau_i, \bar{T}, T_{bound})$  contribution of layer  $i$  to observed radiance  $y$

$\sigma_i = \sum_{j=1}^i \varepsilon_j$ ; contribution of atmosphere above level  $i$  to the observed radiance ( $\sigma_i = y$ )

$u_i$  = absorber amount for layer  $i$

$q_i$  = mixing ratio at boundary  $i$

## Accelerated Numerical Implementation

- Existing "Path Characterization" algorithm (Isaacs et al, 1990) calculates Jacobian by finite differencing on radiances - i.e. computes as many radiances as there are retrieved parameters
- New approach: calculates Jacobian analytically
- Gain in computation is achieved by
  - 1) eliminating the redundancy in the radiative transfer calculations

	Current	New	Gain (for N=20, M=2)*
# of opt. depth calculations	$N + M \times N^{**2}$	$N + M \times N$	~14
# of layer emission calculations	$N + M \times N^{**2}$	$< 2N$	~20**

\* N = number of levels, M = number of constituents (e.g. M=2 for simultaneous retrieval of temperature and water vapor); gain = current/new operations

\*\* Loses roughly a factor 2 over Path Characterization algorithm due to the fact that current code operates at finest DV.

Oden

## Accelerated Numerical Implementation (continued)

---

- 2) efficient vectorization (each step in the radiative transfer calculations operates simultaneously on 2400 spectral elements)
- 3) minimization of I/O's

### PRELIMINARY TIMING FIGURES

Derivative calculations for temperature (at 23 levels) and water vapor (18 levels) - continuous spectral coverage from  $500$  to  $1400 \text{ cm}^{-1}$  at full spectral resolution: 30 min. with old version on Convex at Phillips Lab.(Goal with improved version: <10 min).

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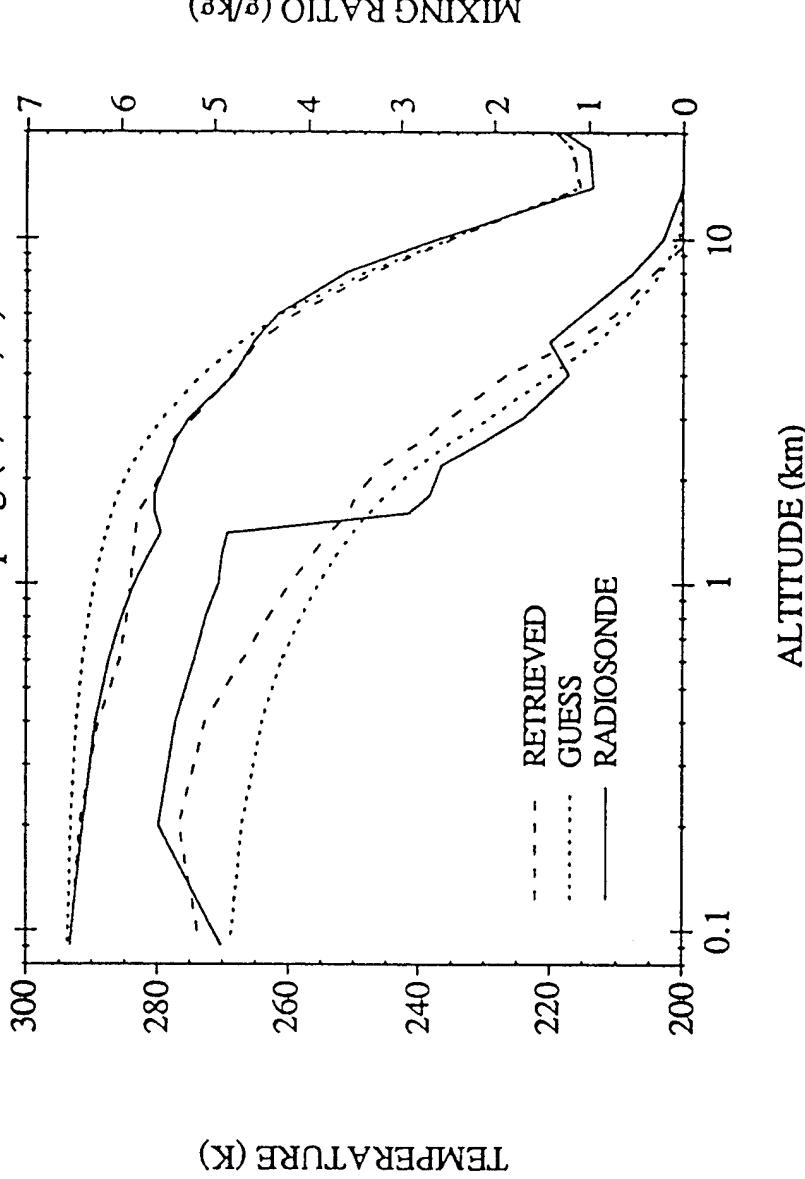
## Examples of Application

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- SIMULTANEOUS RETRIEVAL OF LOW ALTITUDE TEMPERATURE AND WATER VAPOR FROM GROUND BASED IR MEASUREMENTS (DBIS, J.M. Theriault et al., 1993)
- RETRIEVAL OF HIGH ALTITUDE OH PROFILES FROM BALLOON BORNE MICROWAVE SOUNDER (Steve Miller, PL/OS)

dej

SIMULTANEOUS RETRIEVAL SIMULATION:  
Hot Dry Case-jl02a  
709 Channels (2 cm-1 res) : First Guess Estimation :  
Tuned Damping (4, 100, 2)

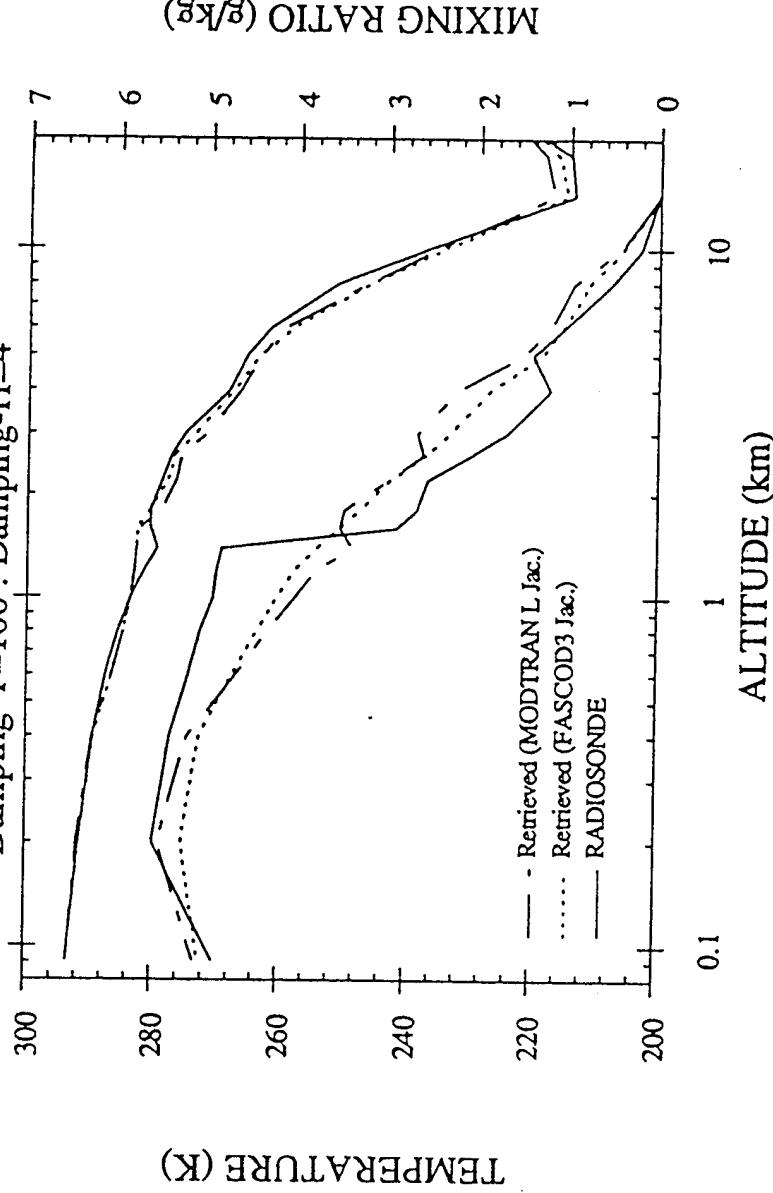


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SIMULTANEOUS RETRIEVAL (ji02a simulation):  
FASCODE / VS / MODTRAN-L JACOBIANS

Spectral Band 500 1400 cm<sup>-1</sup>

Damping-T=100 : Damping-H=4



## Future Work

---

- **Develop limb retrieval capabilities:**
  - already incorporates sphericity and atmospheric refraction
  - explore ways to speed up radiative transfer calculations
- **Extend the code to include cross-sections for heavy molecules**
- **Continue work on user interface**
- **Continue to improve speed:**
  - progressive spectral degradation of the transfer calculations through filtering operation
  - analytical derivations of the Jacobian for molecular mixing ratios and eventually temperature
- **Long term: treatment of clouds and aerosol by coupling the code with CHARTS (Moncet and Clough, 1992)**
- **Parallelization**

Oler

## Acknowledgements

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This work is supported by the U.S. Air Force/Phillips Lab under contract F19628-93-C-0040.

Our thanks to Gail Anderson and Steve Miller of the Optical Science Division of the Phillips Lab for their support and collaboration.

# **SIMULATION OF STELLAR OCCULTATION MEASUREMENTS**

Liisa Oikarinen

Erkki Kyrölä, Elina Sihvola, and Johanna Tamminen

Finnish Meteorological Institute

Department of Geophysics

1. Stellar occultation method
2. GOMOS instrument
3. Atmospheric model
4. Data inversion

## GOMOS = Global Ozone Monitoring by Occultation of Stars

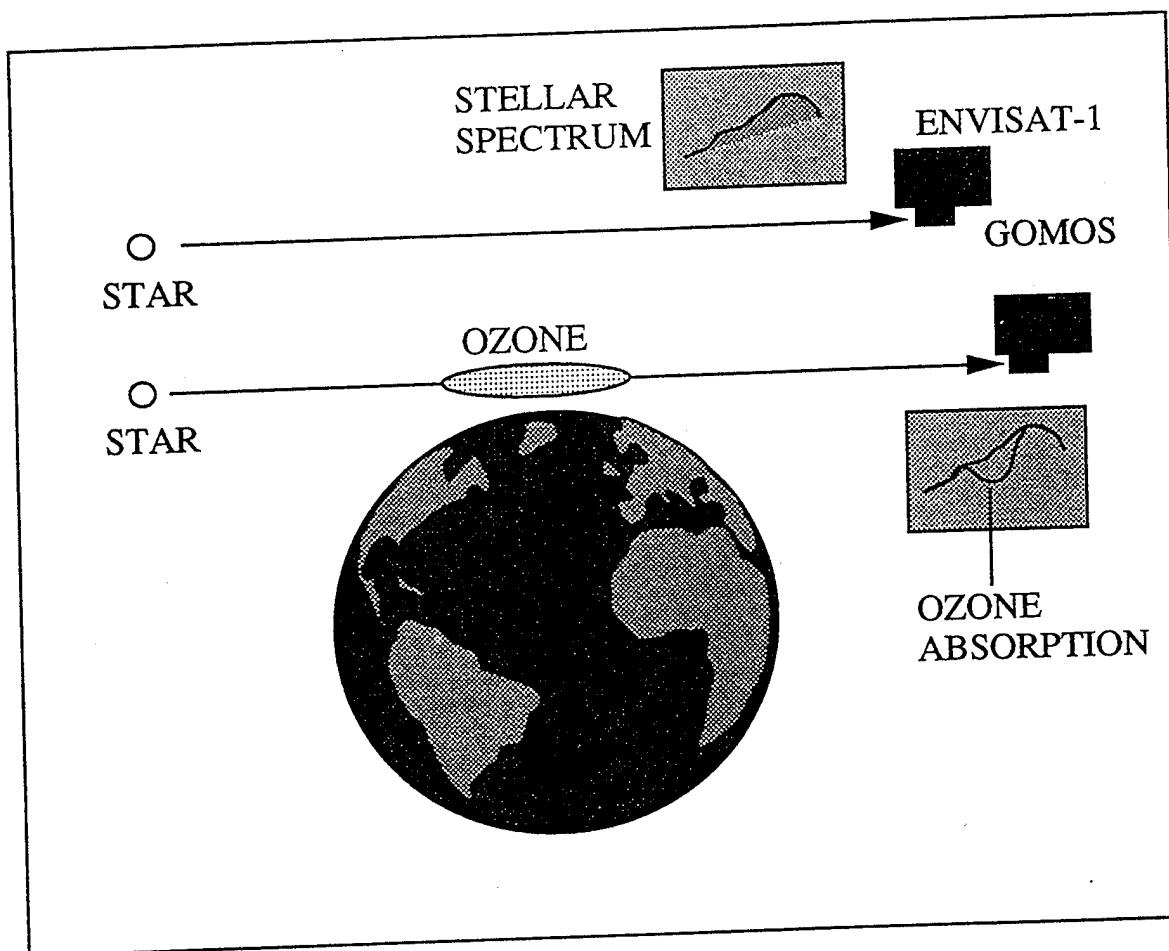
- An ESA Developed Instrument (EDI), funded under the ENVISAT-1 programme
- Main objective of GOMOS: trend studies of ozone
- Measurement: global mapping of stratospheric O<sub>3</sub>, NO<sub>2</sub>, NO<sub>3</sub>, aerosols, H<sub>2</sub>O, temperature (O<sub>2</sub>)
- Launch 1998

## Role of FMI in GOMOS:

- Scientific help in instrument development
- Development of data retrieval methods
- Data center



## The stellar occultation measurement principle



Tangent height 15 - 100 km

Vertical resolution 2 km (CCD integration time 0.5 s)

Stars up to magnitude 4 are used (bright limb up to 2)

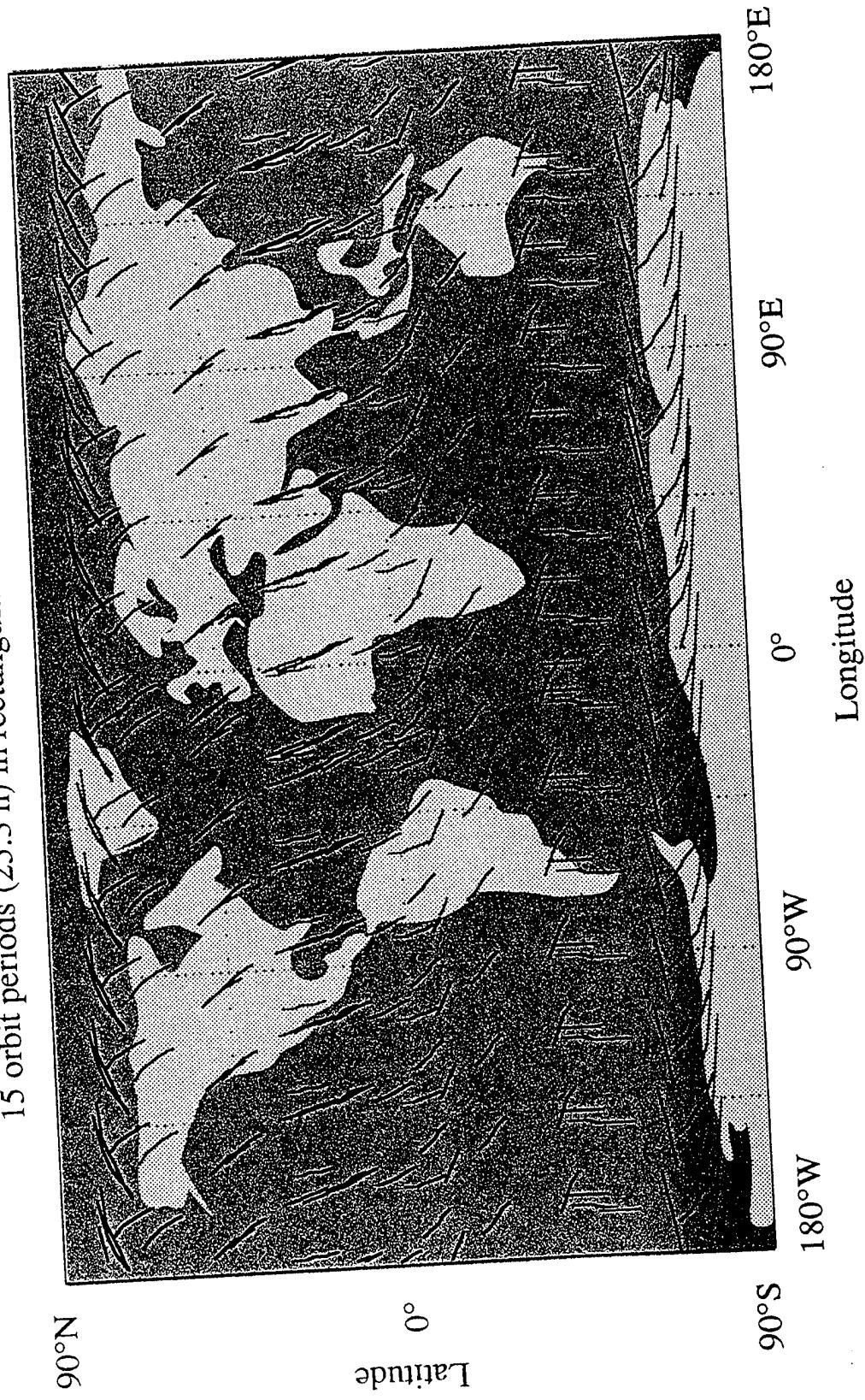
Heliosynchronous polar orbit, altitude 800 km

Nominal orbit period 100 min

25 - 40 occultations per orbit

## Global coverage of GOMOS measurements

15 orbit periods (25.3 h) in rectangular co-ordinates, in March



# GOMOS INSTRUMENT

## UVIS-spectrometer:

- Large spectral width: 250 - 675 nm,  
both Chappuis and UV-bands can be exploited:  
ozone can be retrieved at 15 - 90 km
- A good spectral resolution (1 nm), i.e., many pixels:  
Counteracts faintness of stars;  
Several trace gases can be retrieved: O<sub>3</sub>, NO<sub>2</sub>, NO<sub>3</sub>, ...
- Two dimensionality of CCD:  
Solar scattered background can be measured,  
daytime measurements feasible;  
Pointing errors counteracted;  
Refractive bending counteracted

## IR-spectrometer:

- O<sub>2</sub> and H<sub>2</sub>O measurement (756 - 773 and 926 - 952 nm,  
0.06 nm resolution)
- From O<sub>2</sub> neutral density and temperature to support  
UVIS-analysis

## Photometers:

- 470 - 520 nm and 650 - 700 nm, maximum sampling  
rate 1 kHz
- Measurement of scintillations: The stellar signal can be  
corrected
- Studies of turbulence

## Why stellar occultation?

- Calibration stability
- Global coverage
- Altitude resolution

### Solar occultation - SAGE

- + relative measurement
- only two occultations per orbit
- night/day terminator measurements
- + good altitude resolution (1 km)

### SBUV-TOMS, TOVS

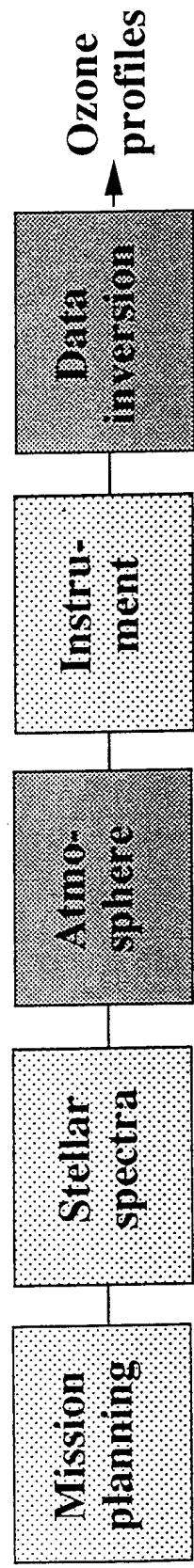
- absolute measurement
- + good coverage
- only dayside measurements
- poor altitude resolution (8 km)



### Stellar occultation-GOMOS

- + relative measurement
- + global coverage (night and day)
- + sufficient altitude resolution (2 km)

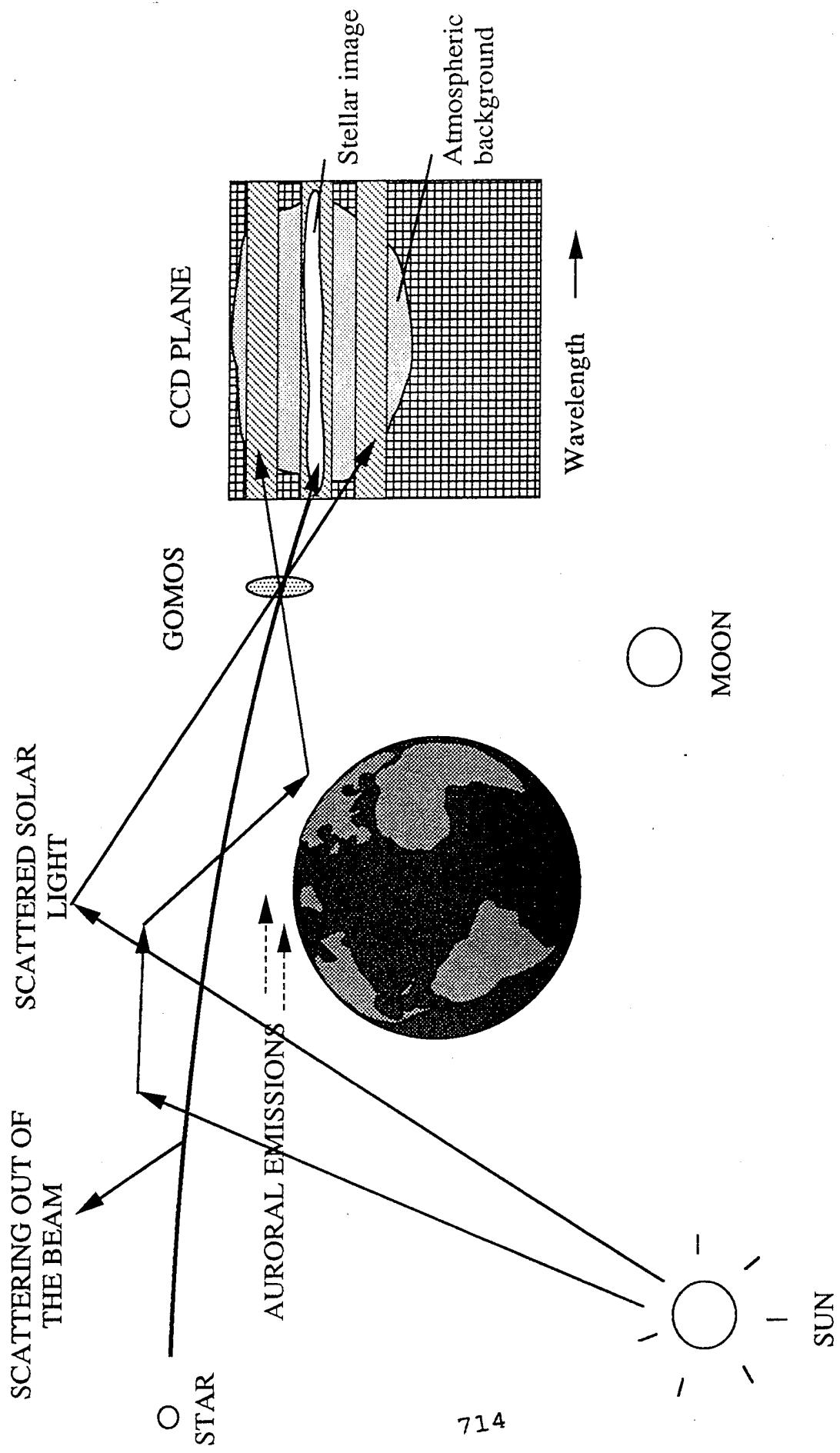
## GOMOS simulation

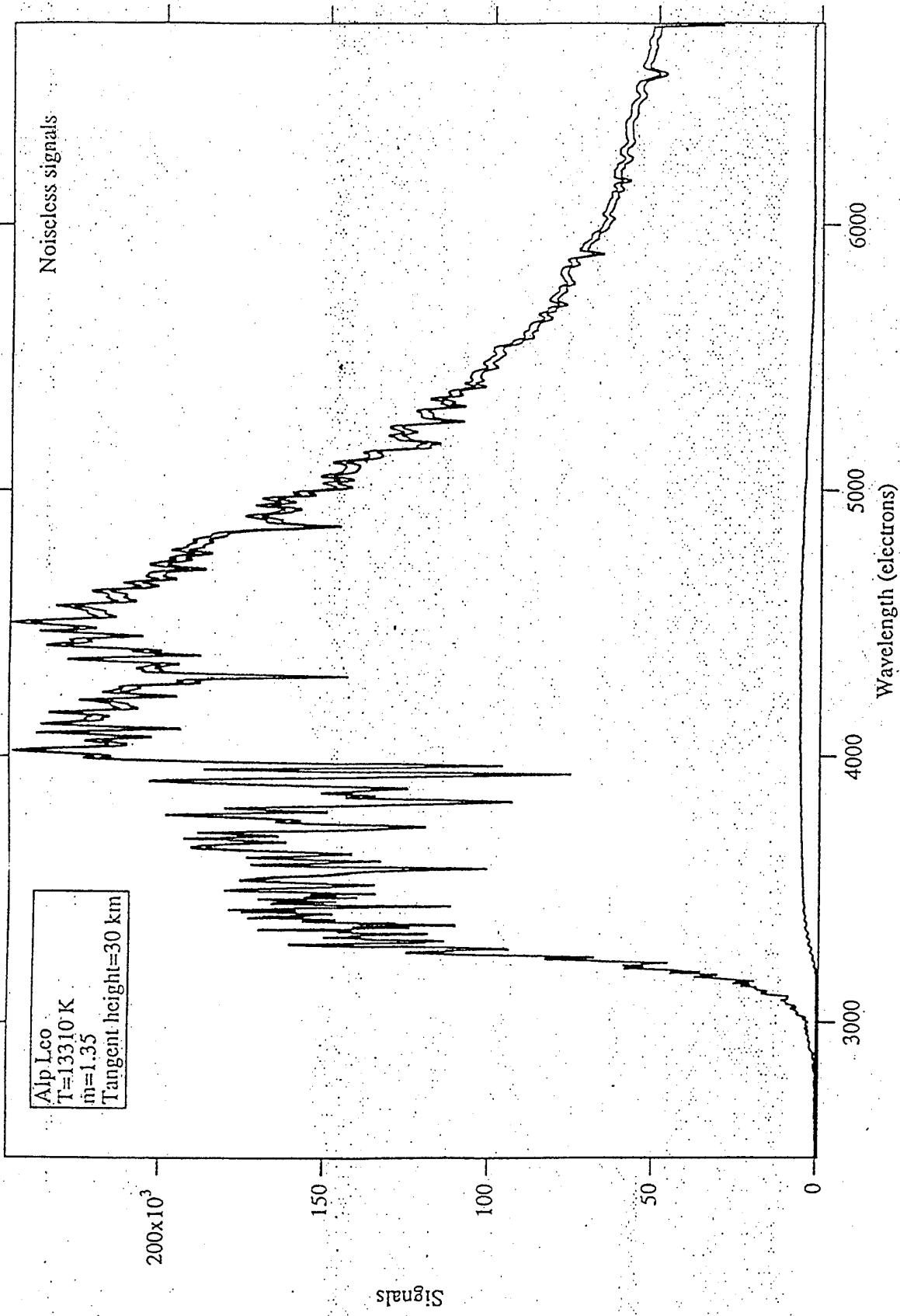


## ATMOSPHERIC PHYSICS FOR GOMOS

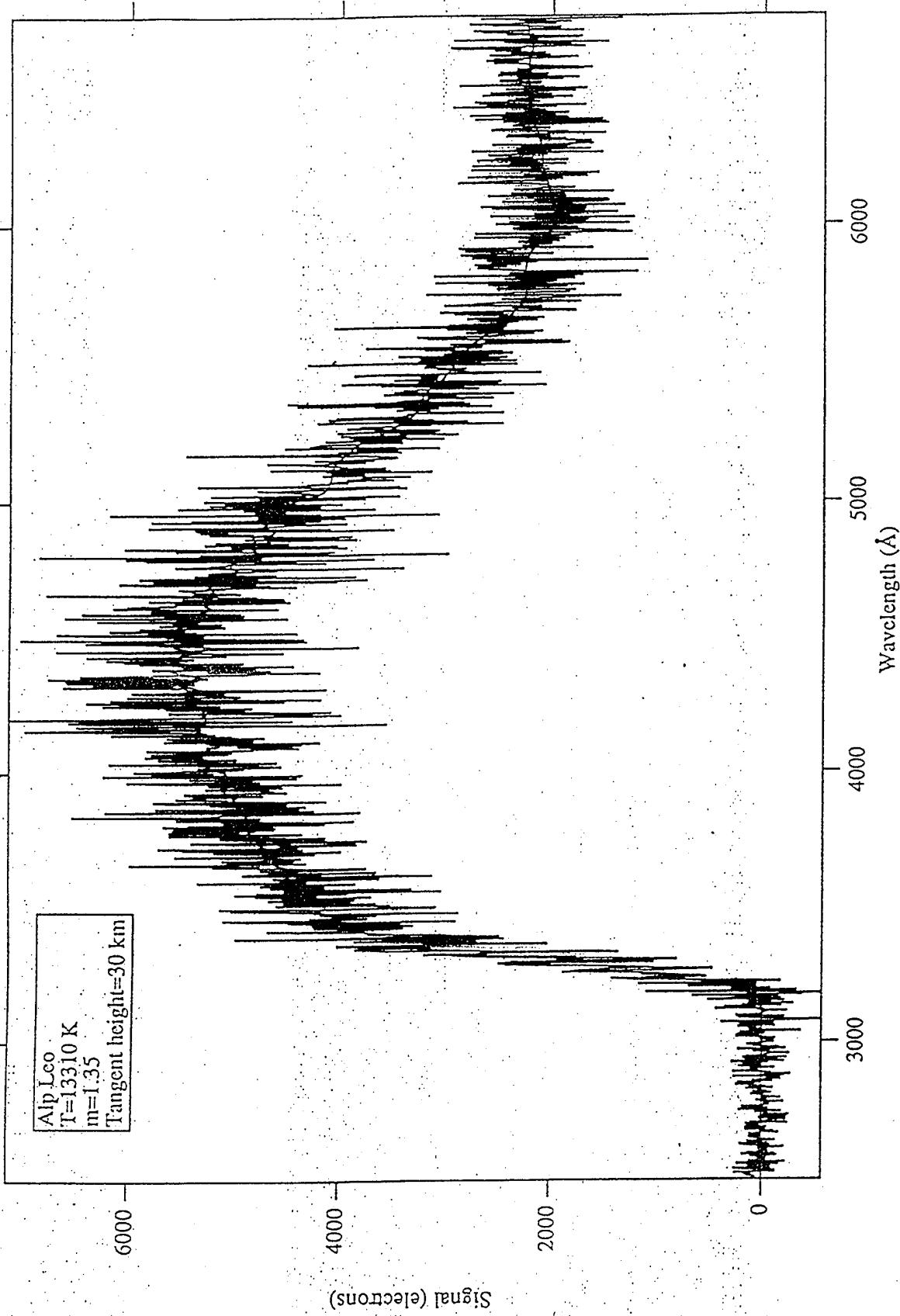
Phenomena that should be simulated:

- Absorption by  $O_3$ ,  $NO_2$ ,  $NO_3$ ,  $OCIO$ ,  $SO_2$ ,  
 $BrO$ ,  $H_2O$ ,  $O_2$
- Scattering out of the beam by Rayleigh and  
aerosol scattering
- Scattering of solar light by molecules and aerosols  
into the FOV of the instrument
- Emission into the FOV (aurora etc.)
- Refraction: bending of the ray, refractive attenuation
- Turbulence: scintillations





Alp Lco  
 $T=13310\text{ K}$   
 $m=1.35$   
Tangent height=30 km

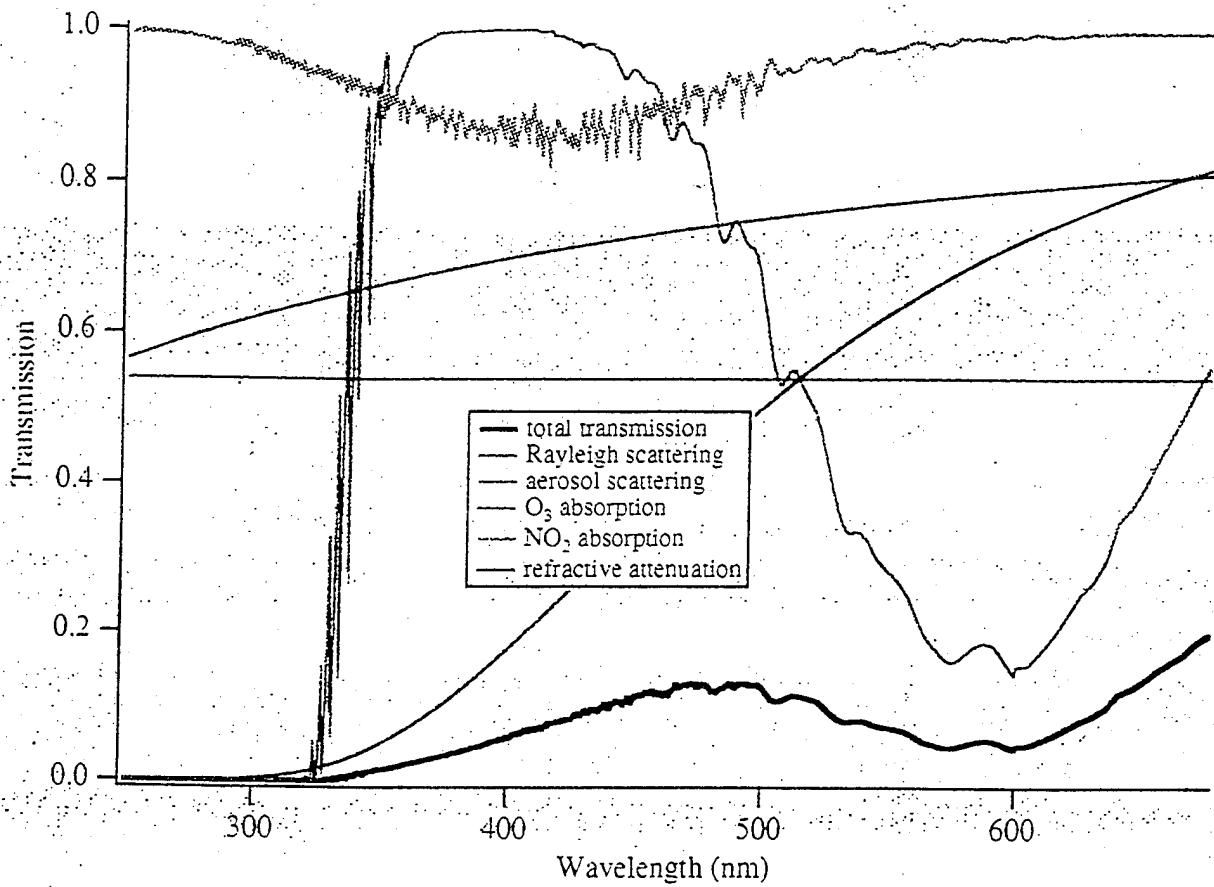


## SPECIAL REQUIREMENTS OF GOMOS ATMOSPHERIC SIMULATION MODEL

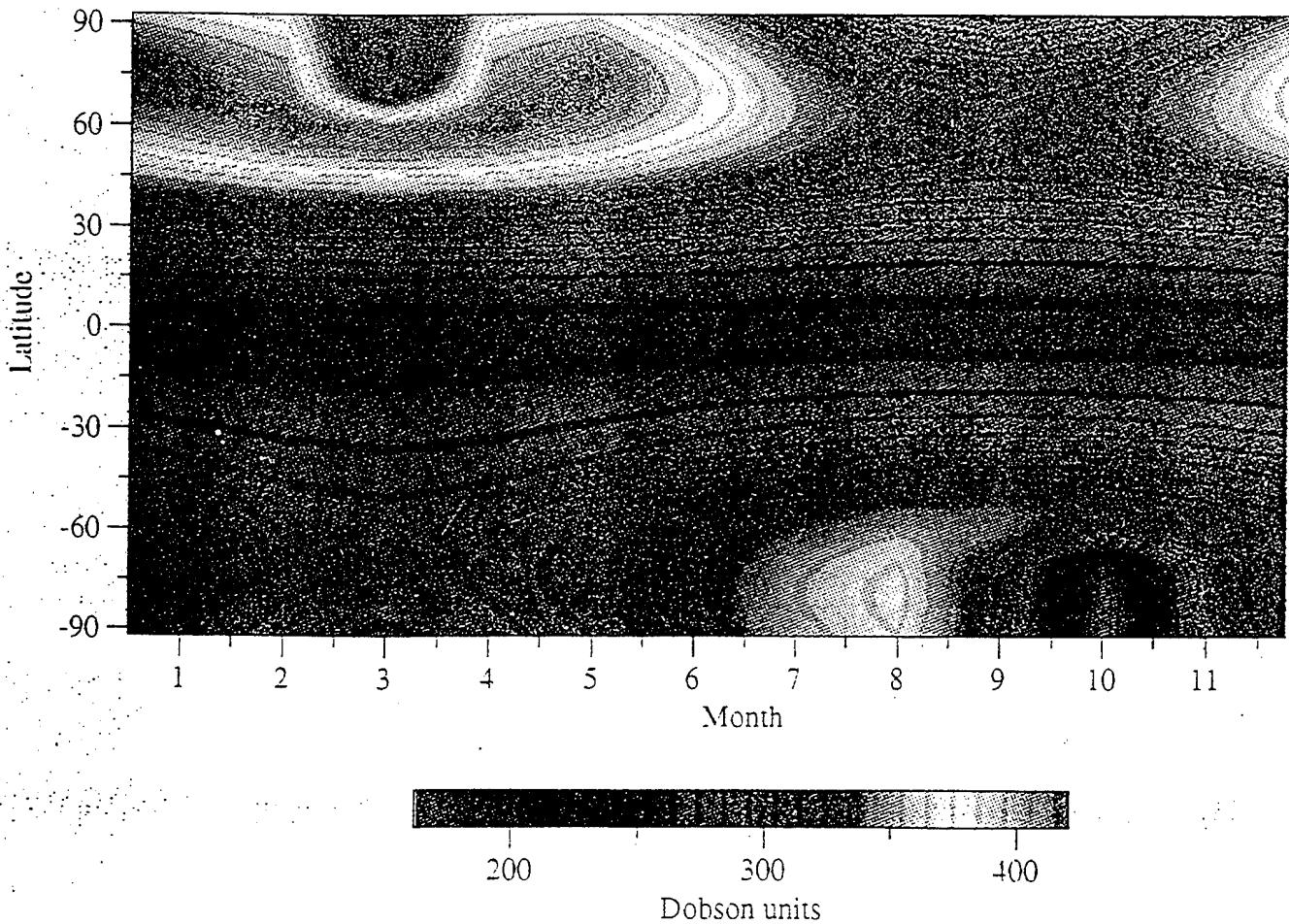
- compactness (analytical density distributions etc.)
- the code should be easy to modify
- realistic variations in constituent distributions  
(ultimate conditions, eg. the ozone hole, required in addition to average atmospheres)
- occultation geometry

Comparison of FINGOM (a code specially designed for GOMOS by FMI) and LOWTRAN

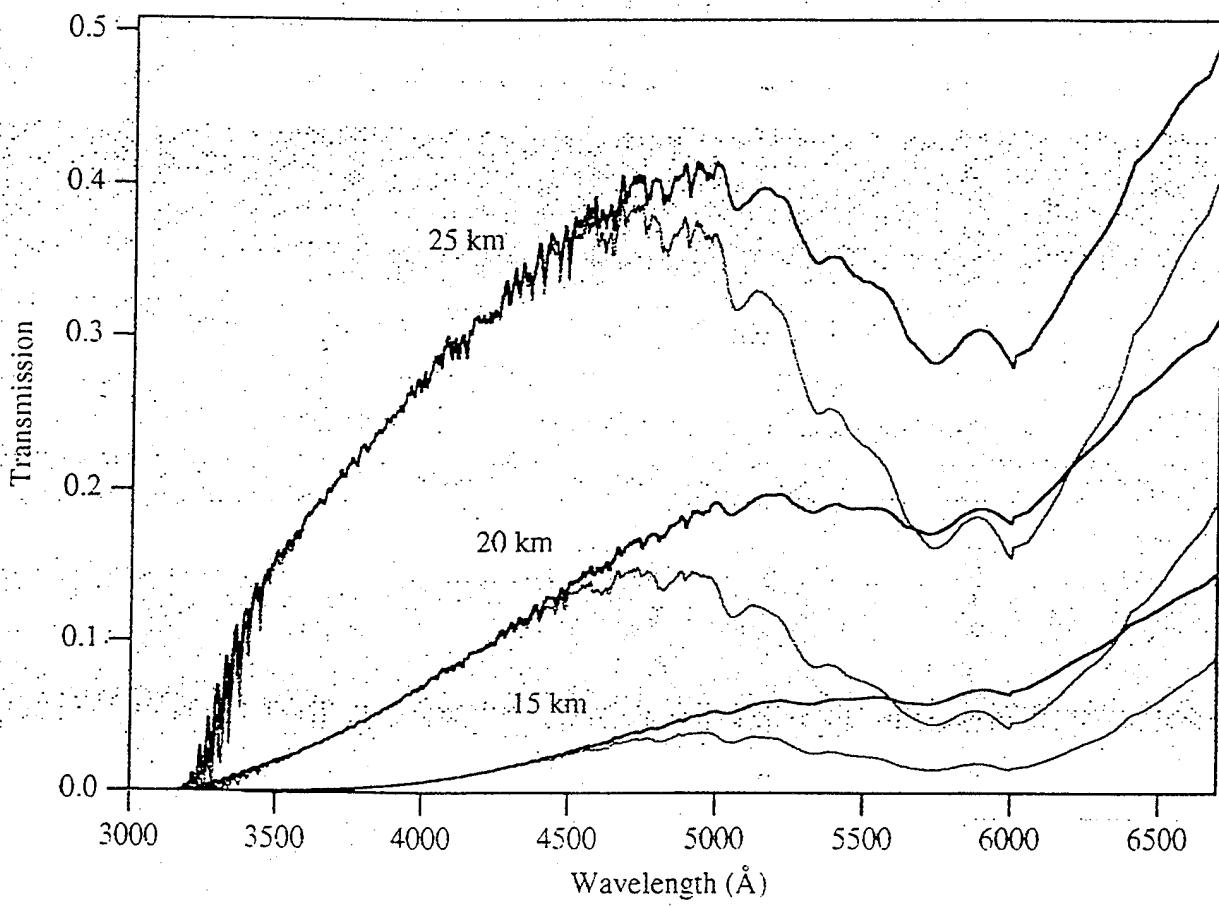
model	FINGOM	LOWTRAN
absorbers in the vis.	O <sub>3</sub> , NO <sub>2</sub> , NO <sub>3</sub> , SO <sub>2</sub> , BrO, OCIO	O <sub>3</sub>
constituent profiles	3-D, seasonal, diurnal, latitudinal variations	local geographical-seasonal atmospheres
atmospheric model description	analytic	tables
refractive attenuation	included	not included
scattered solar background	single scattering	single- and multiple scattering
aerosol model	simple	models for various aerosol conditions



Atmospheric transmission for a ray path of tangent height 20 km. Total transmission is divided into the main extictive components  $T_{\text{tot}} = T_{O_3} T_{\text{Rayl}} T_{\text{aer}} T_{NO_2} T_{\text{refr.}}$



Total ozone distribution model as a function of latitude and season.



# INVERSION

$$T(l) = e^{-\tau(\lambda, l)}$$

$$\tau(\lambda, l) = \int k(\lambda, s) ds = \int \sum_i \rho_i(s) \sigma_i(\lambda, T(s)) ds$$

Discretization:

$$(1) \quad 1^\circ \quad \tau(\lambda, l) = \sum_i N_i(l) \sigma_i(\lambda, T_i(l))$$

The same temperature  $T(l)$  is used for the whole ray  $l$

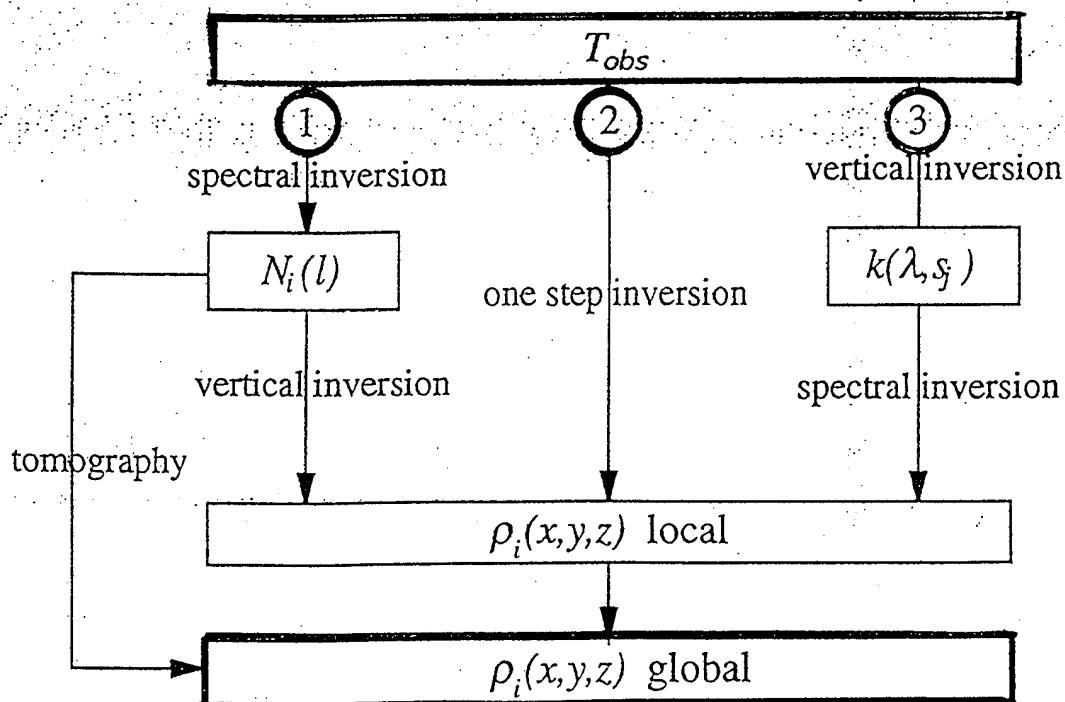
$$2^\circ \quad N_i(l) = \sum_j \rho_i(s_j) \Delta s_j; \quad N_i = \text{line density of constituent } i$$

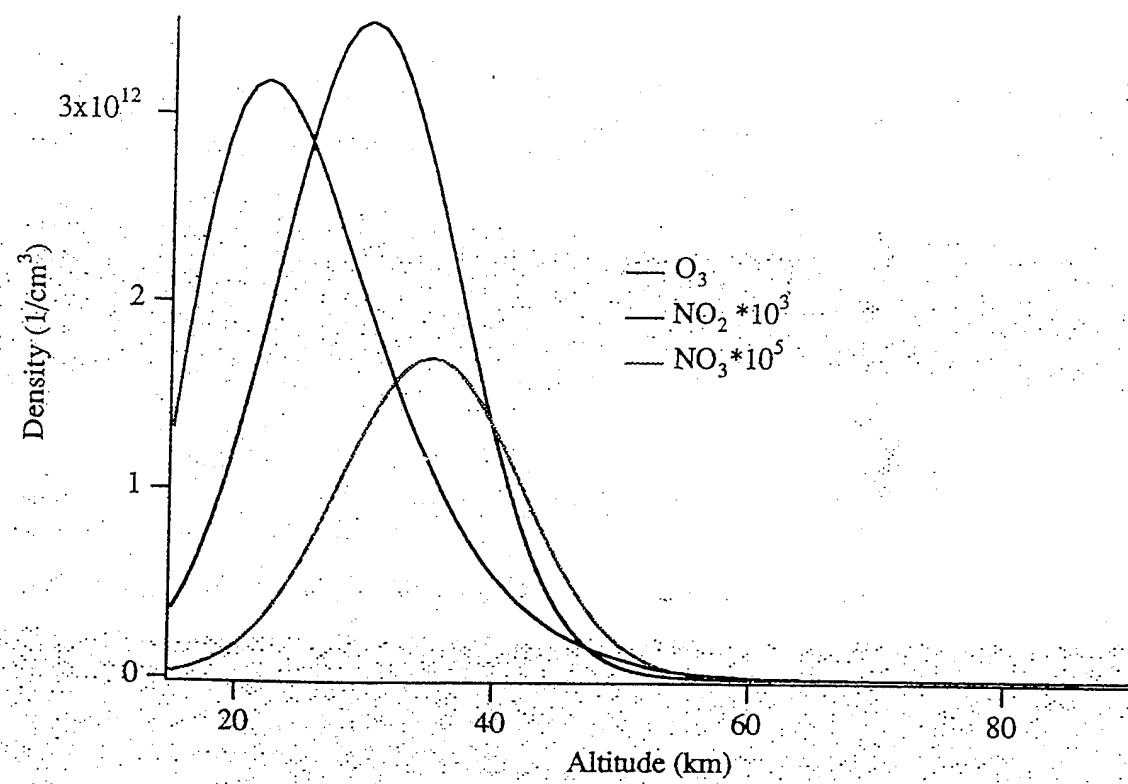
The atmosphere is discretized into layers  $j$

$$(2) \quad \tau(\lambda, l) = \sum_i \sum_{j \in l} \rho_i(s_j) \sigma_i(\lambda, T(s_j)) \Delta s_j$$

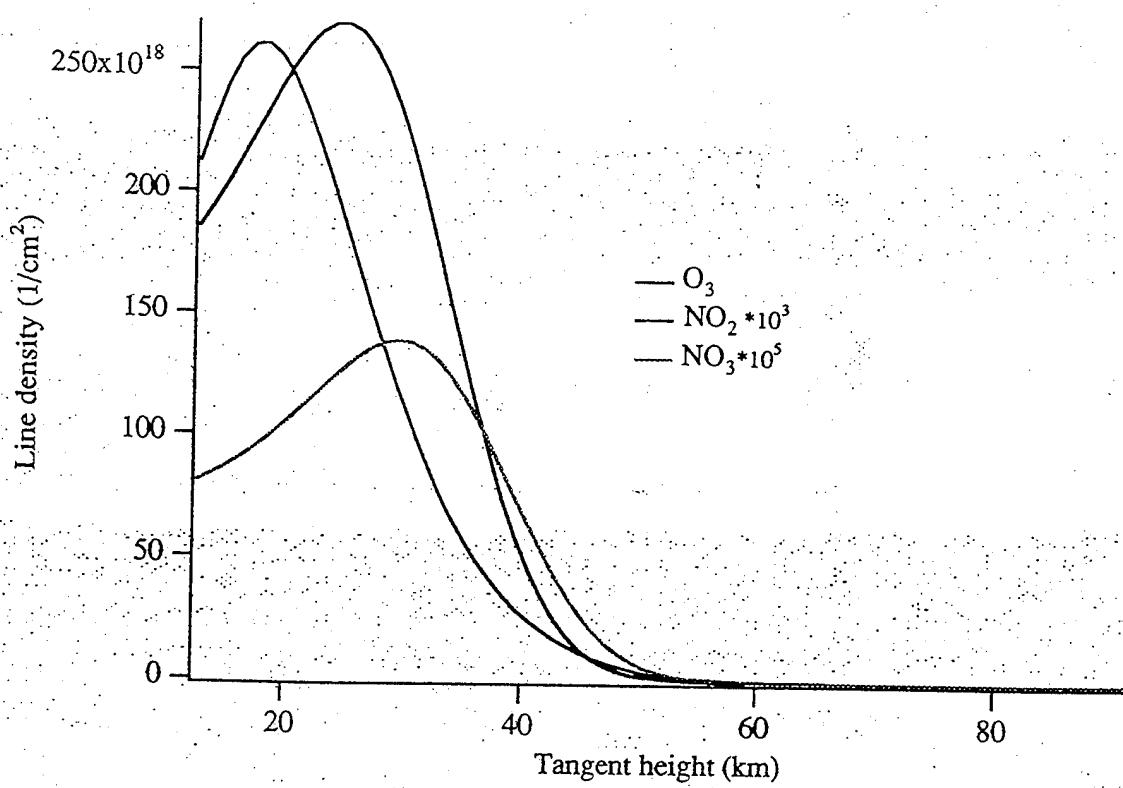
$$(3) \quad 1^\circ \quad \tau(\lambda, l) = \sum_{j \in l} k(\lambda, s_j) \Delta s_j$$

$$2^\circ \quad k(\lambda, s_j) = \sum_i \rho_i(s_j) \sigma_i(\lambda, T(s_j))$$

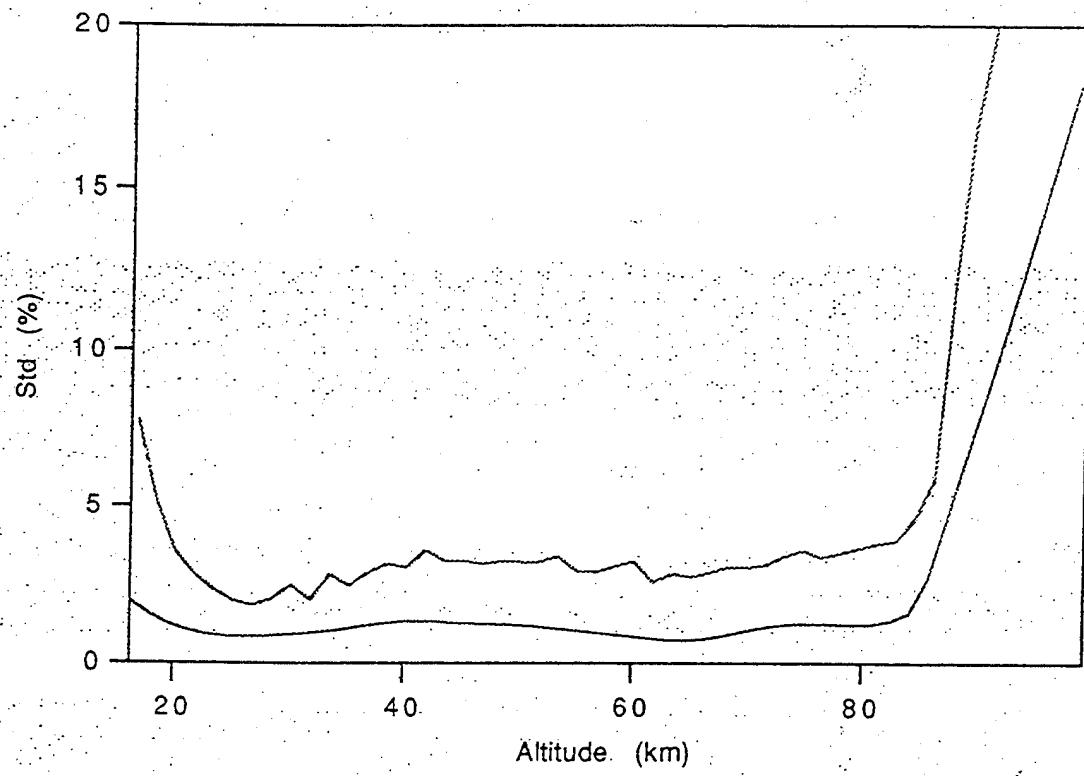




Ozone, NO<sub>2</sub>, and NO<sub>3</sub> density profiles.



Integrated line density for ozone,  $NO_2$ , and  $NO_3$  as a function of the tangent height of the path.



The standard deviation in vertical inversion (upper line). The lower line is the std in the data.

## CONCLUSIONS

An atmospheric model with analytical density distributions has been constructed at FMI.

Realistic simulations of occultation measurements are possible with the model.

### Problems:

- 3-D time dependent models are difficult to construct from the existing data  
(exception: O<sub>3</sub> and temperature)
- Absorber cross-sections are required at 160-280 K, not available at the moment

### Open points:

- simulation of scintillations
- simulation of auroral emissions

der

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**Line by Line Calculation of Atmospheric Fluxes and Cooling Rates:  
Application to Water Vapor, Carbon Dioxide, Ozone, Methane, Nitrous Oxide,  
and the Halocarbons**

**S. A. Clough, and M. J. Iacono  
Atmospheric and Environmental Research, Inc.**

## **Overview/Objectives**

### **Line-by-line Model**

- LBLRTM, (Line By Line Radiative Transfer Model)
- Vectorizable, 10-20x faster (based on FASCODE)
- Extensively validated against observed spectral radiance data (HIS)

### **Water Vapor, Carbon Dioxide, and Ozone:**

- Mid-latitude summer, Mid-latitude winter, Tropical atmospheres
  - Calculate line-by-line upwelling, downwelling, and net (up-down) clear-sky fluxes at 5 cm<sup>-1</sup> resolution for the full IR spectrum (10-3000 cm<sup>-1</sup>)
  - Cooling rates computed from the divergence of the net flux
  - Current US standard profiles used for H<sub>2</sub>O and O<sub>3</sub>; CO<sub>2</sub> = 355 ppm
- Doubled carbon dioxide considered for CO<sub>2</sub> = 710 ppm

### **CH<sub>4</sub>, N<sub>2</sub>O, and the Halocarbons**

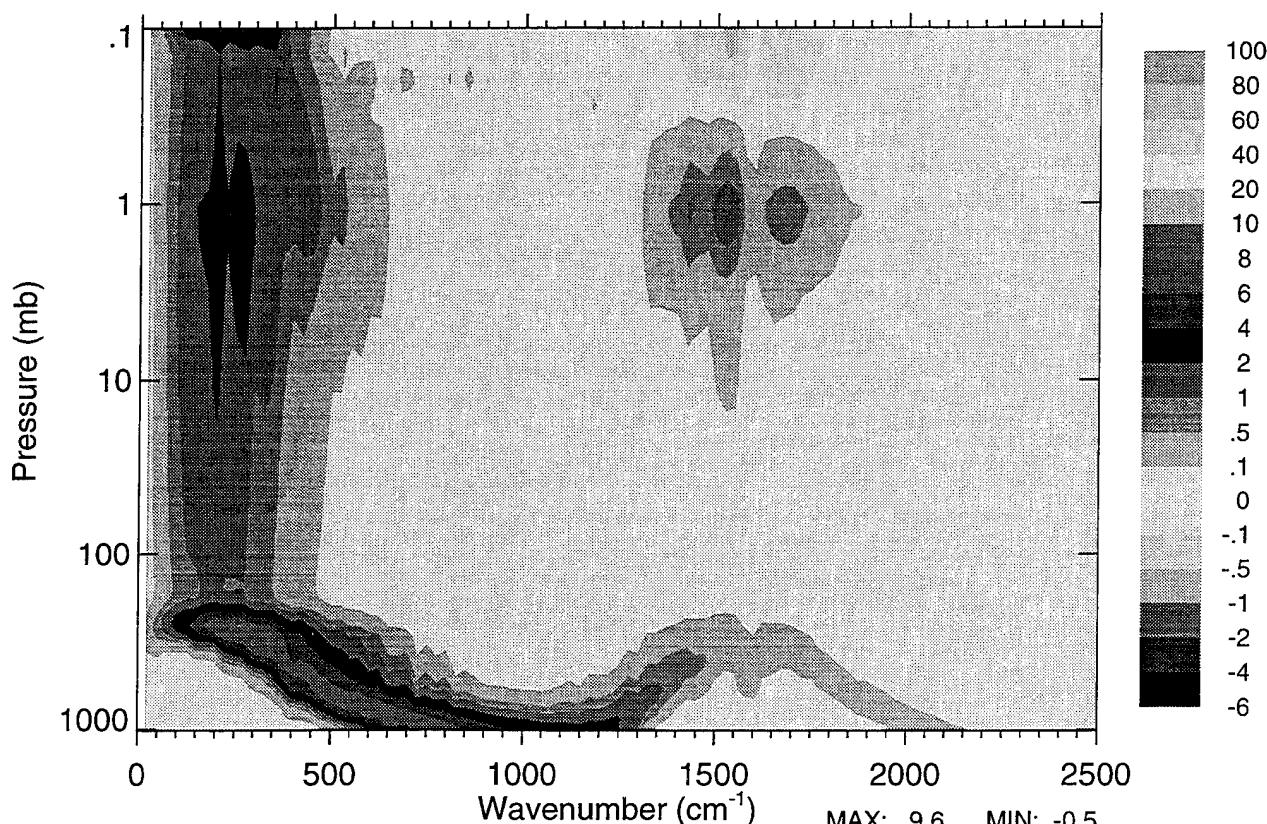
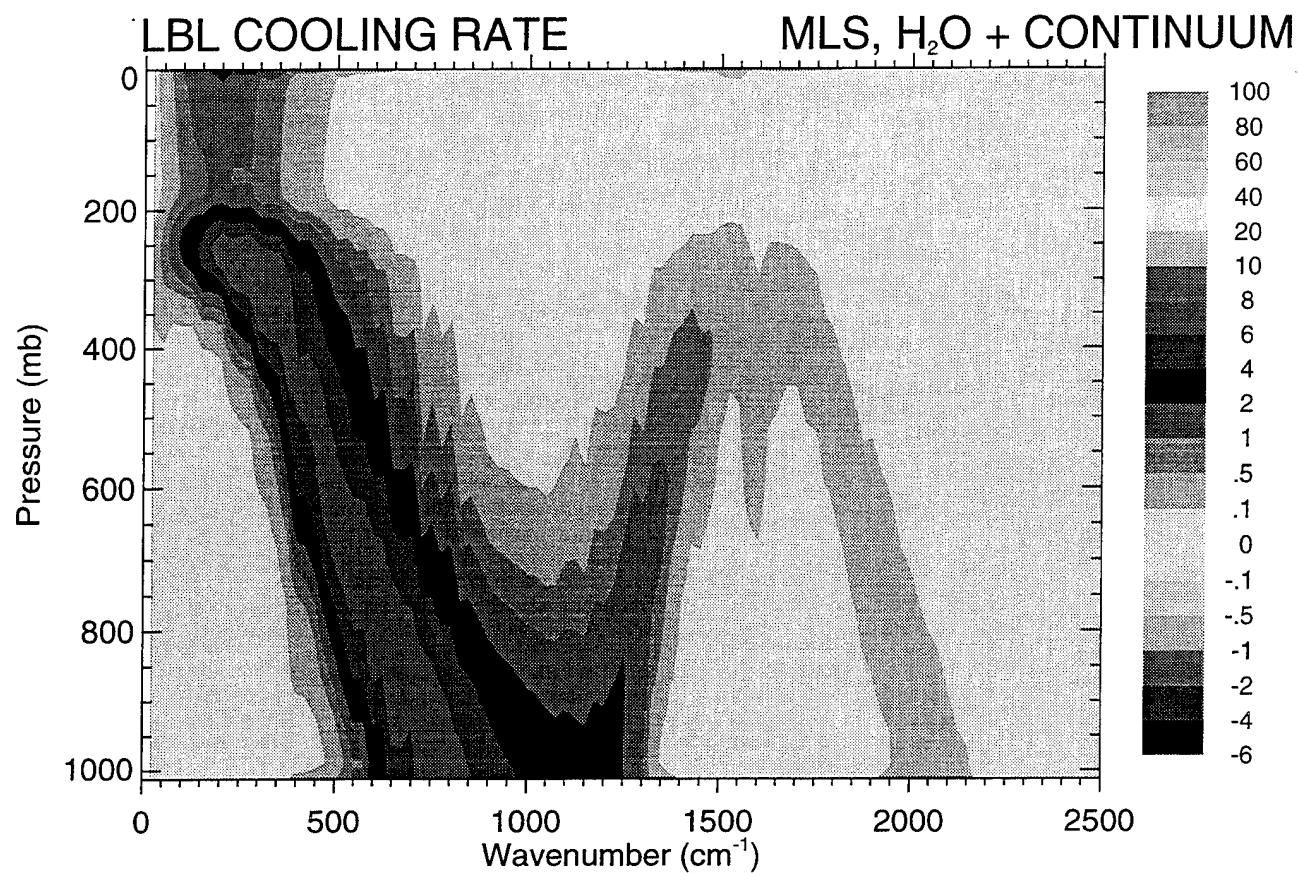
- Halocarbons considered include CFC-11, CFC-12, CFC-22, and CCL4
- Profiles for Methane, Nitrous Oxide, and Halocarbons derived from a 2D chemistry model

### **1990-2000 Changes**

- Ten-year profile changes in all trace species considered for their impact on fluxes and cooling rates
- Changes in water vapor have not been considered

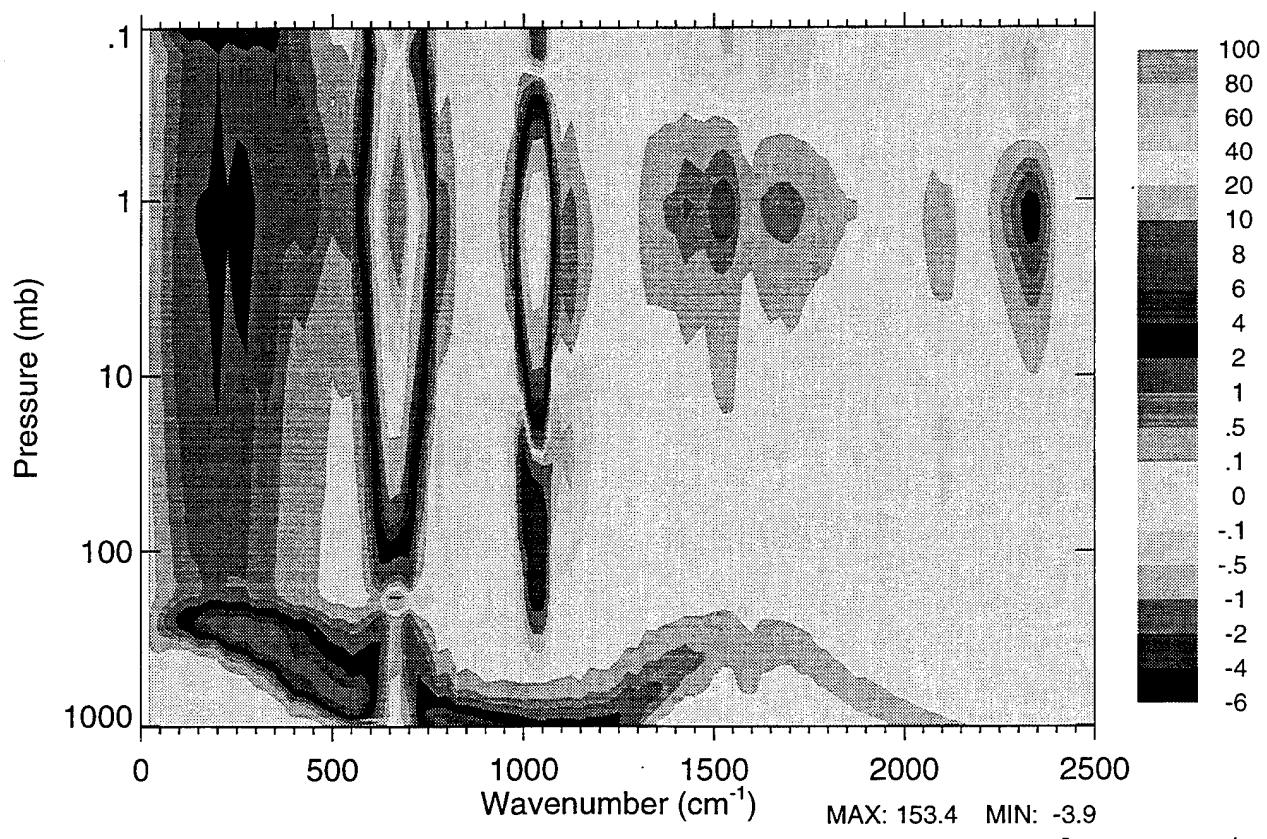
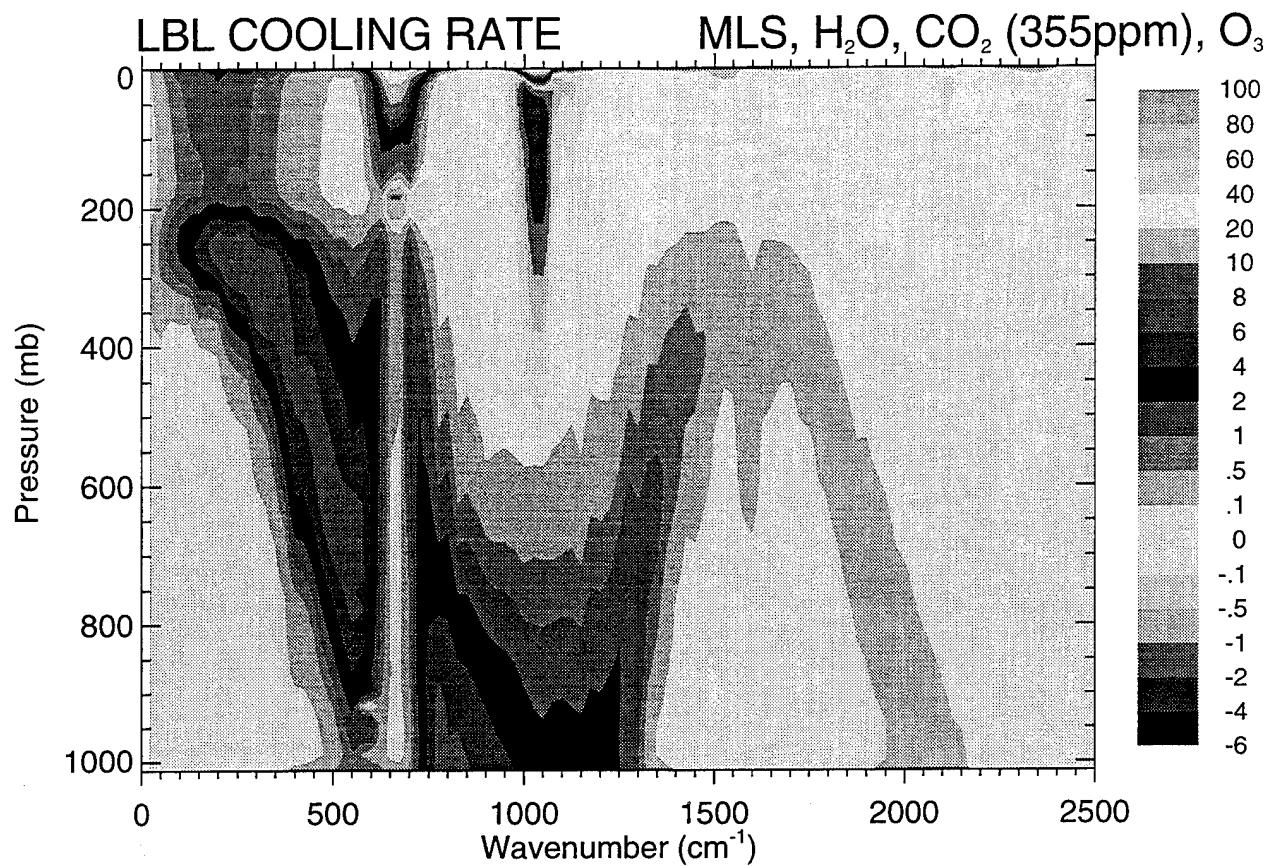
### **Rapid Radiative Transfer Model**

- Apply LBL flux and cooling rate results to the selection of appropriate spectral bands for use in k-distribution model and the verification of the rapid model output.



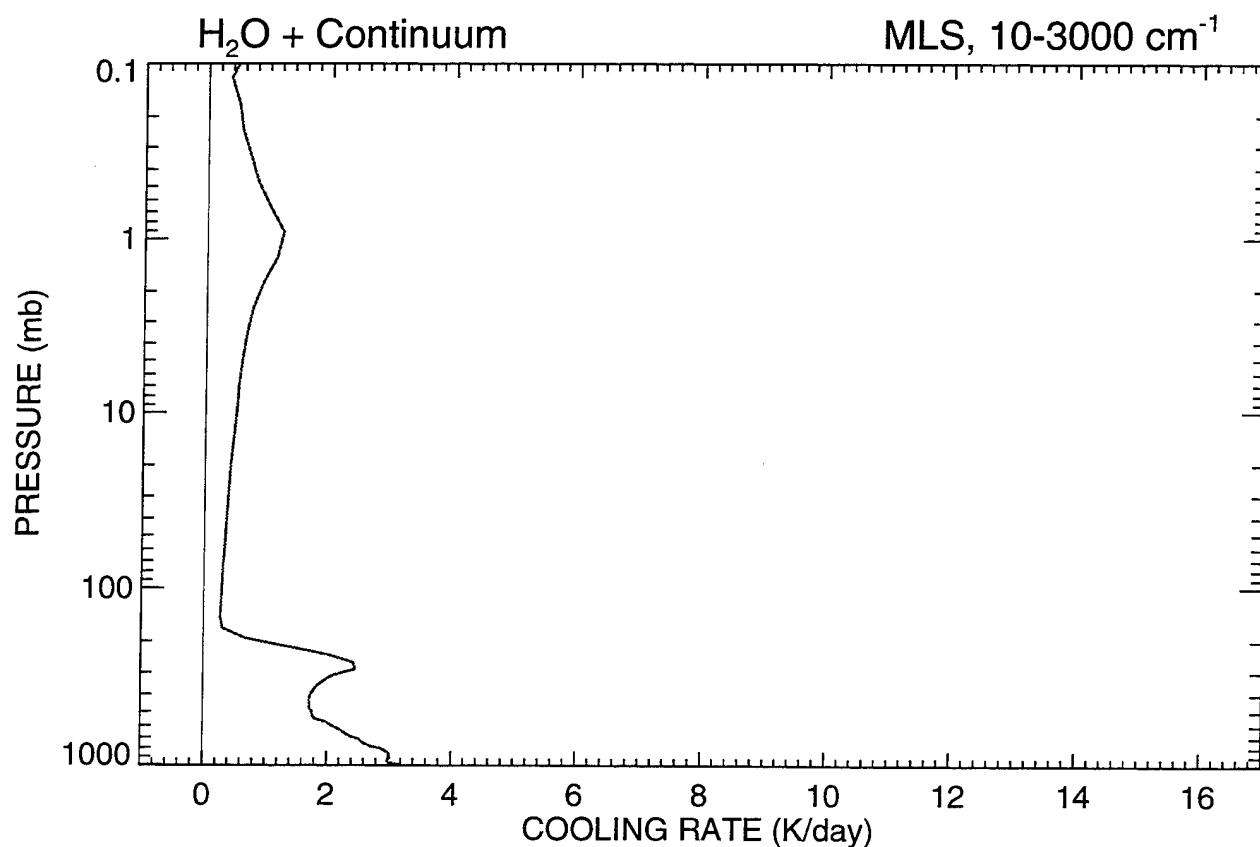
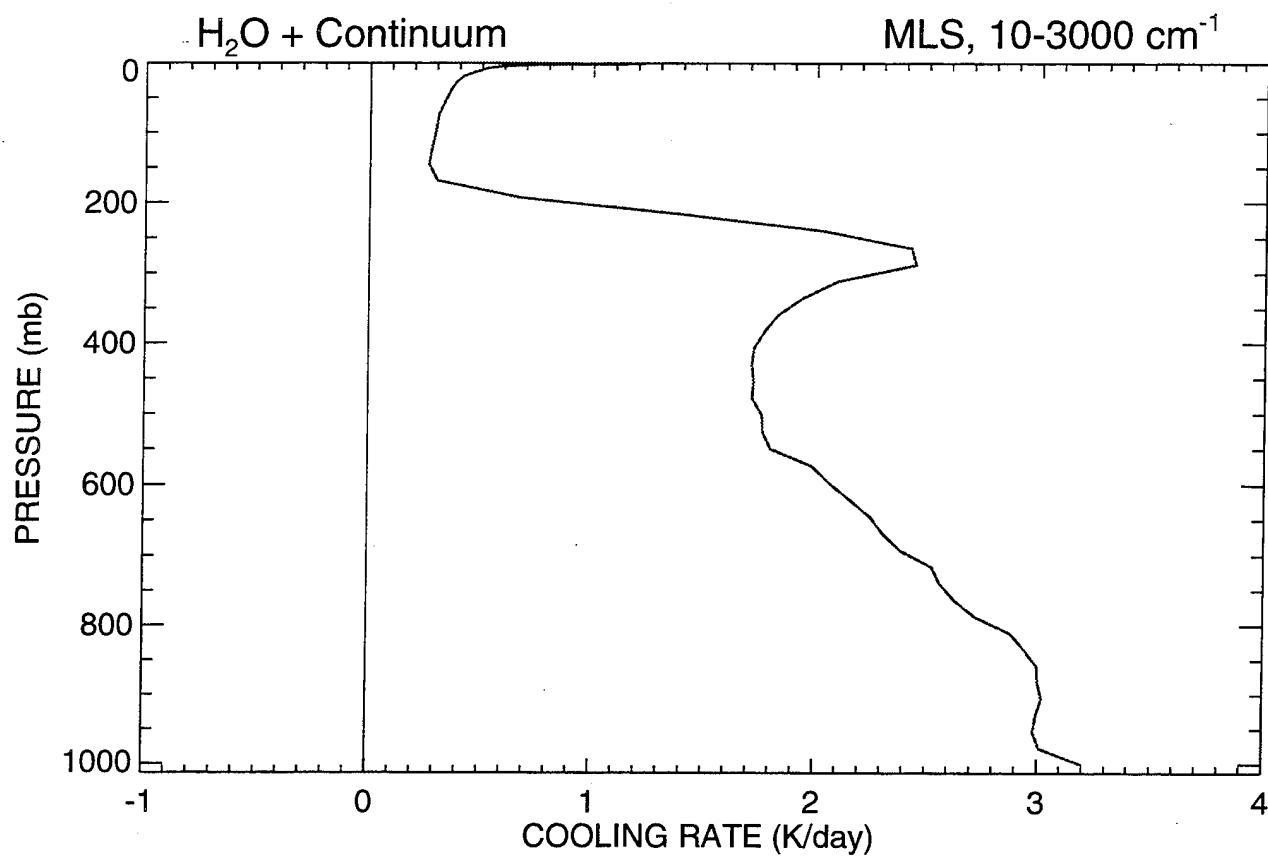
Scale:  $\times 10^{-3} \text{ K}/(\text{day cm}^{-1})$

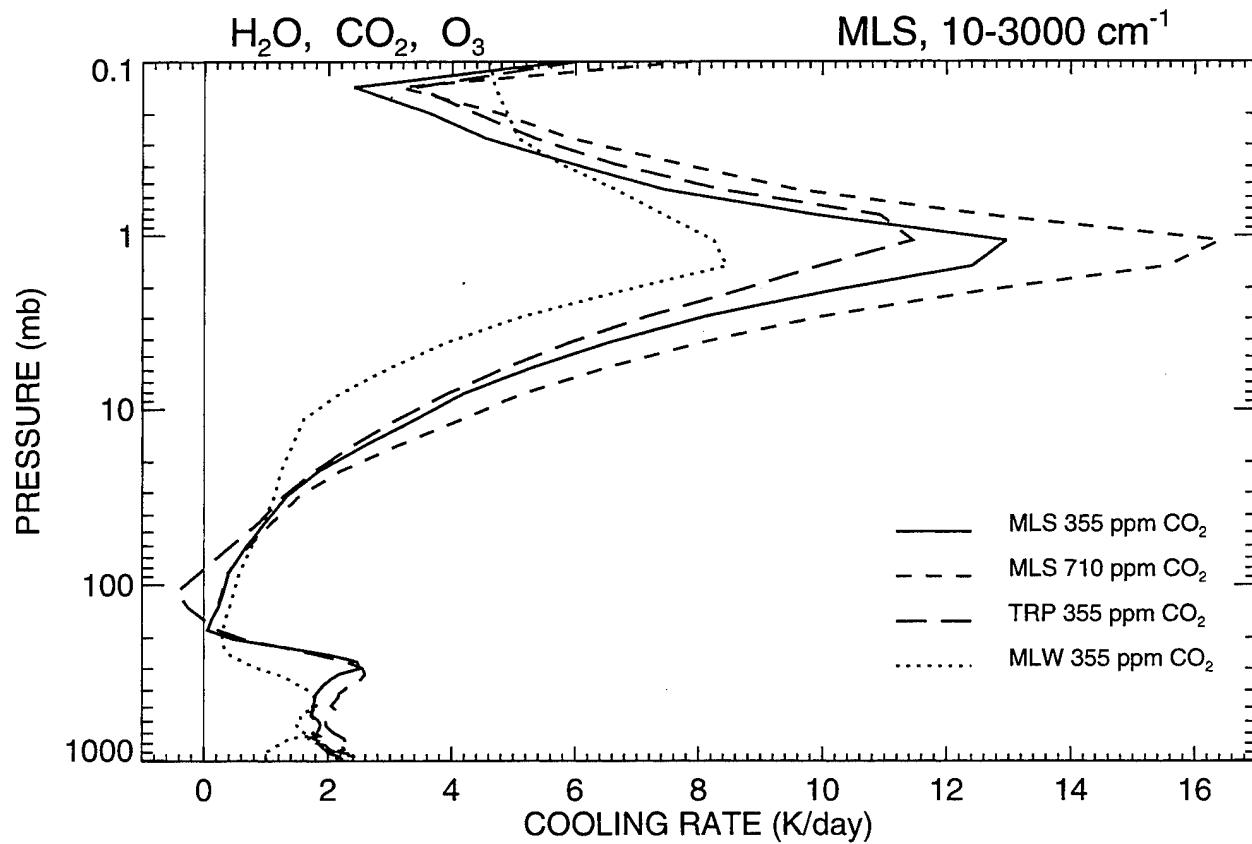
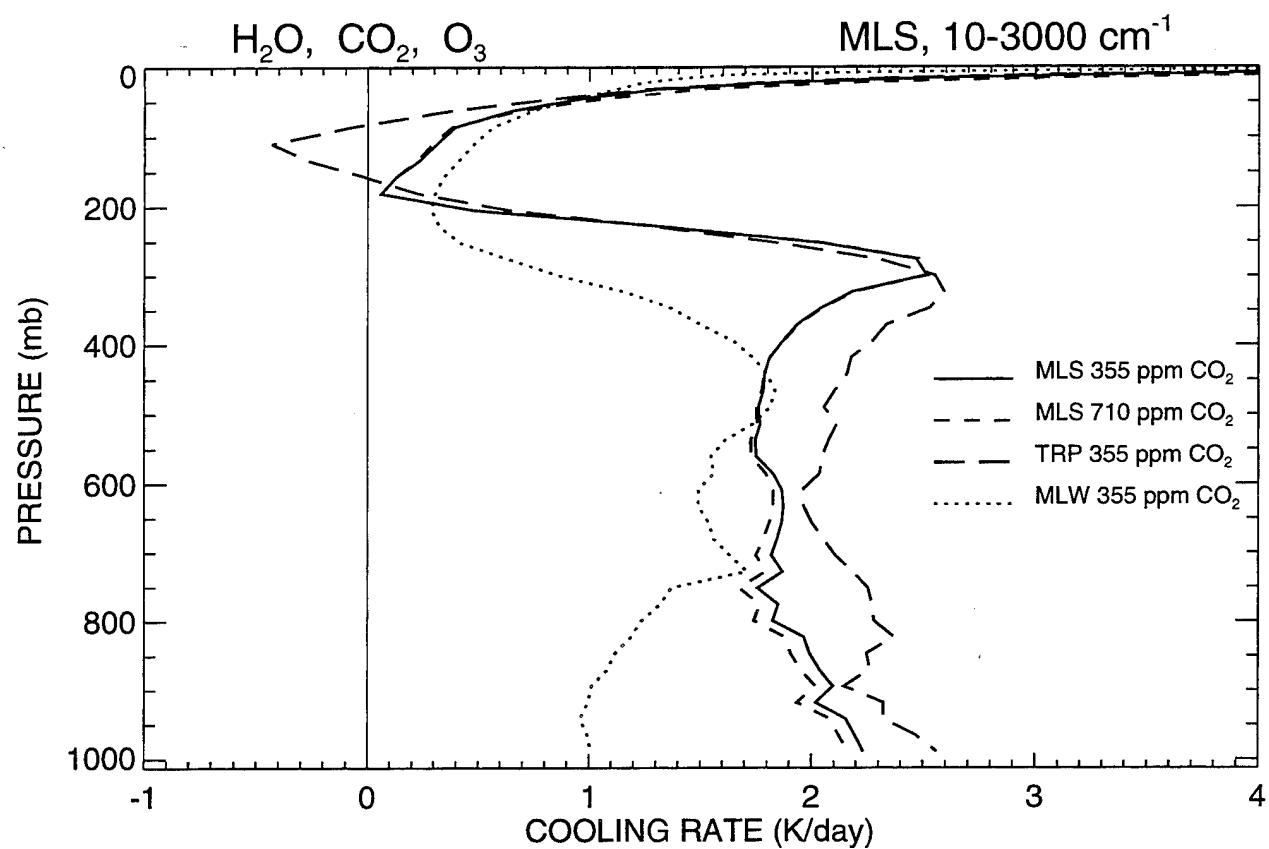
Shepard A. Clough, and Michael J. Iacono  
Atmospheric and Environmental Research, Inc.

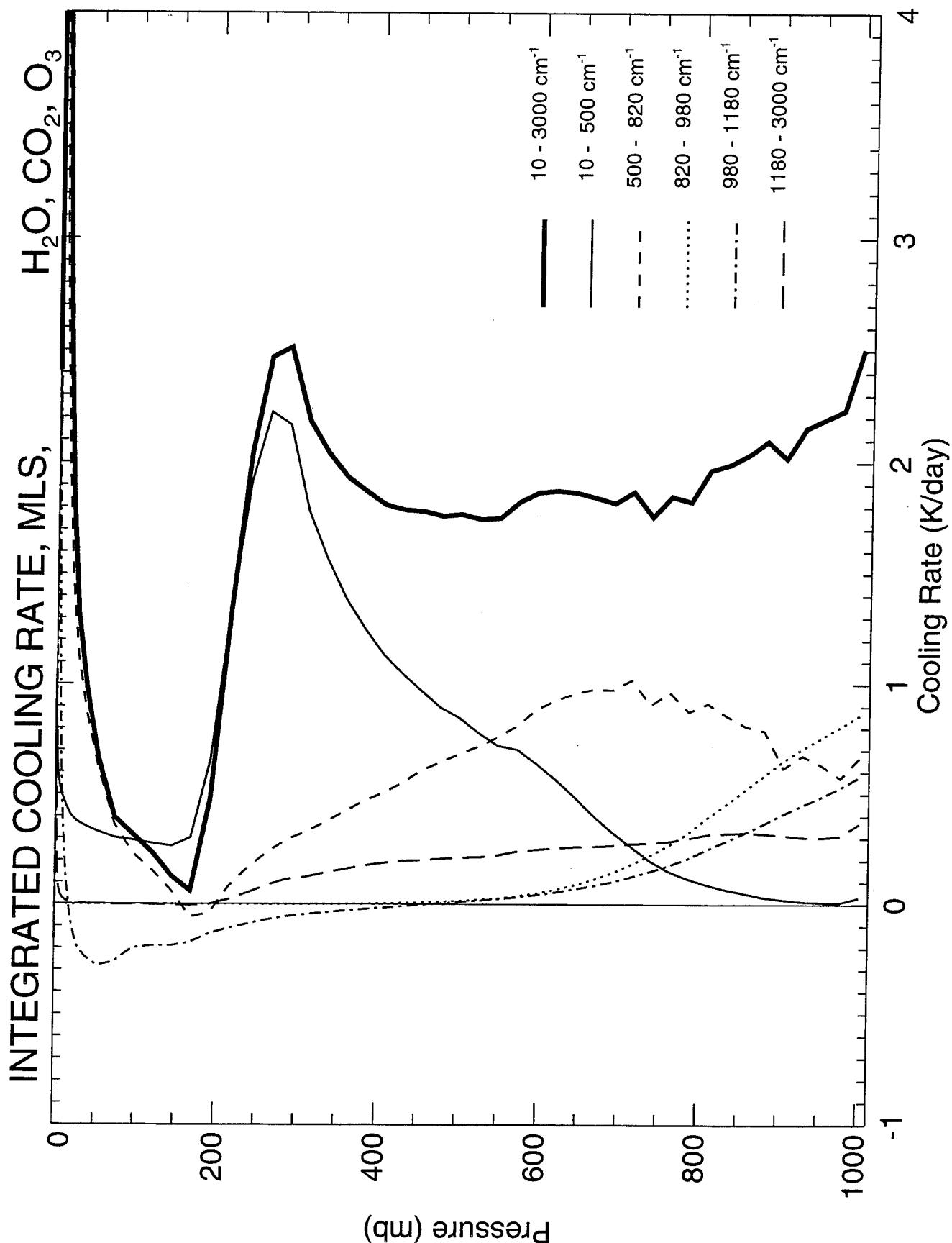


Shepard A. Clough, and Michael J. Iacono  
Atmospheric and Environmental Research, Inc.

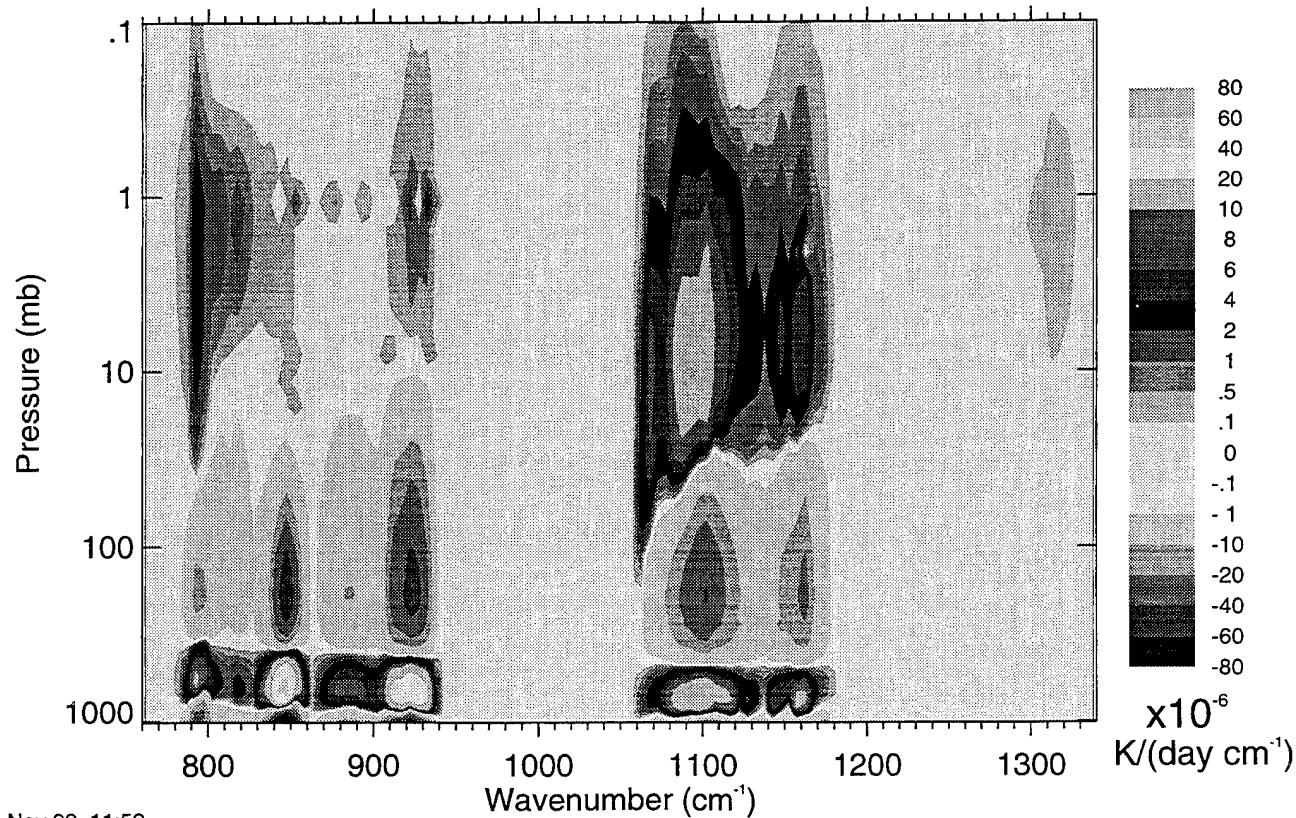
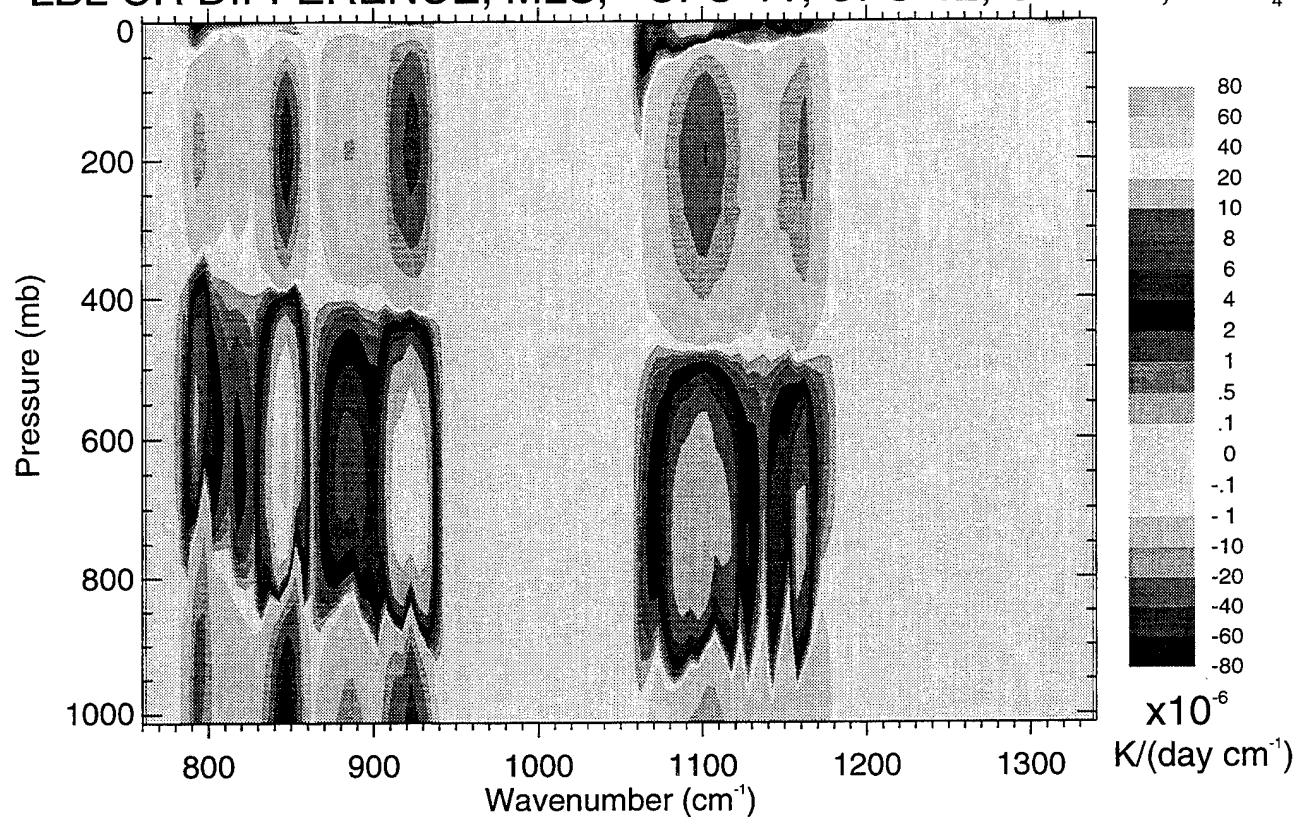
Scale:  $\times 10^{-3}$  K/(day cm<sup>-1</sup>)



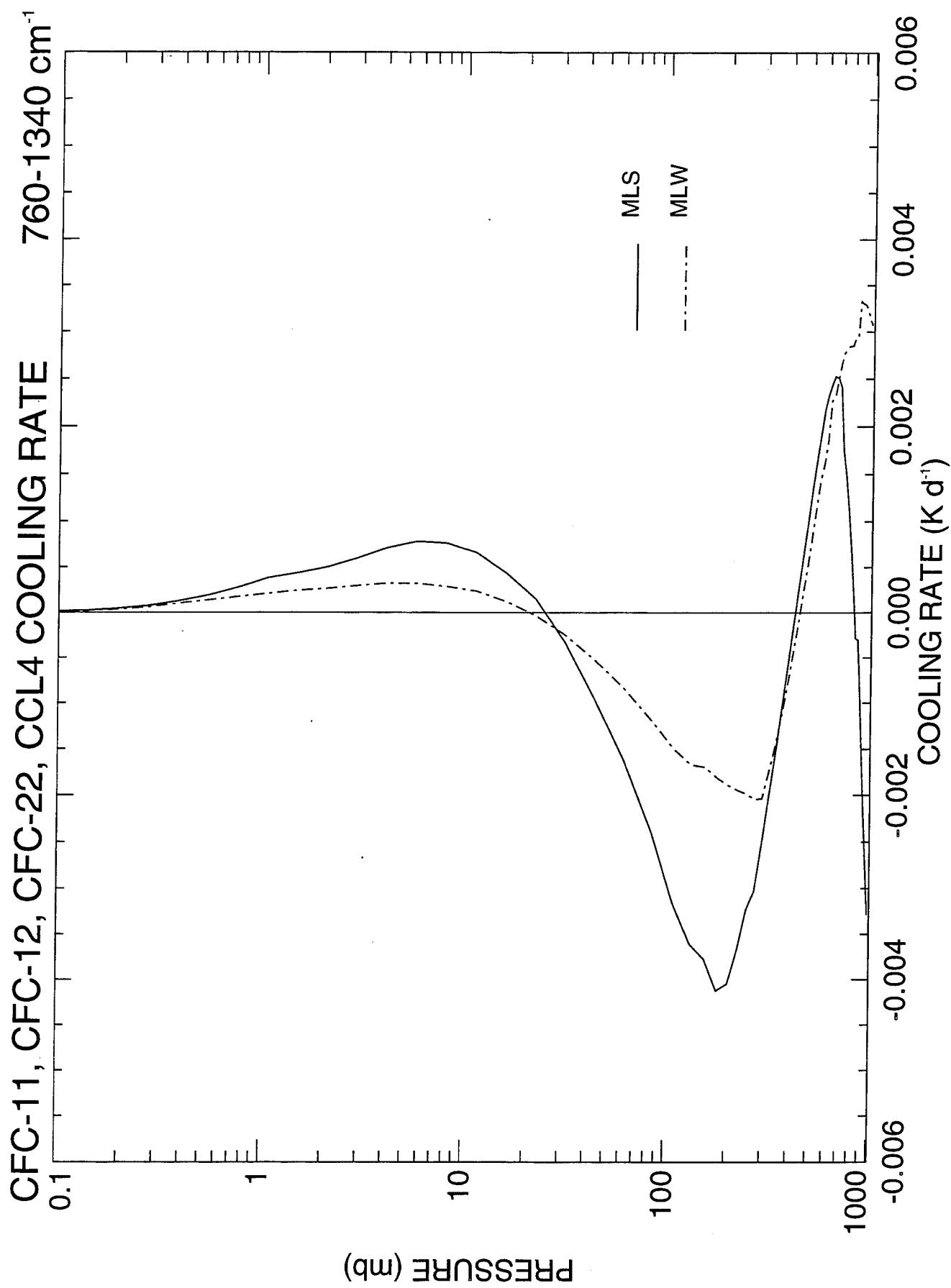




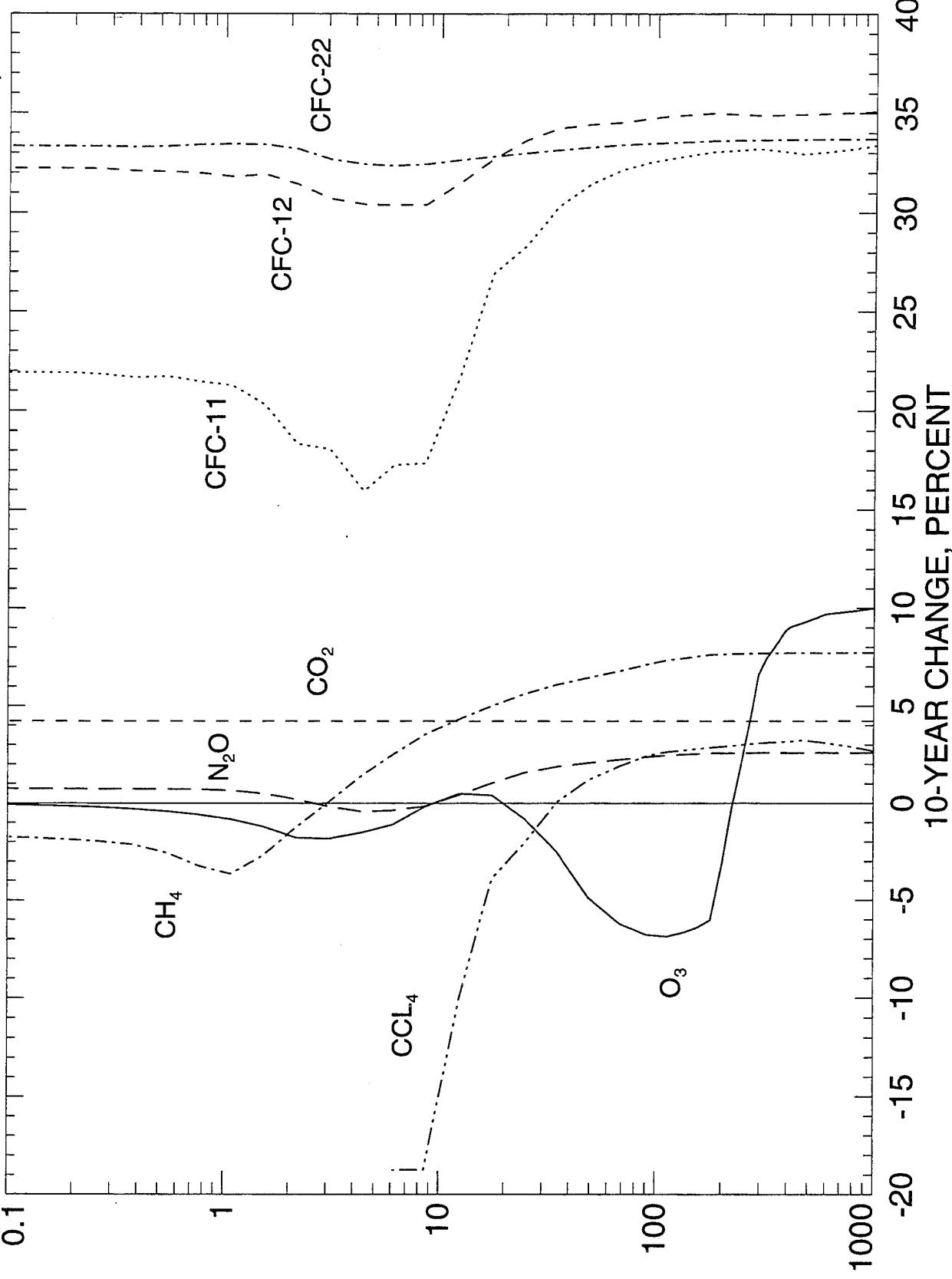
LBL CR DIFFERENCE, MLS, CFC-11, CFC-12, CFC-22, CCL<sub>4</sub>

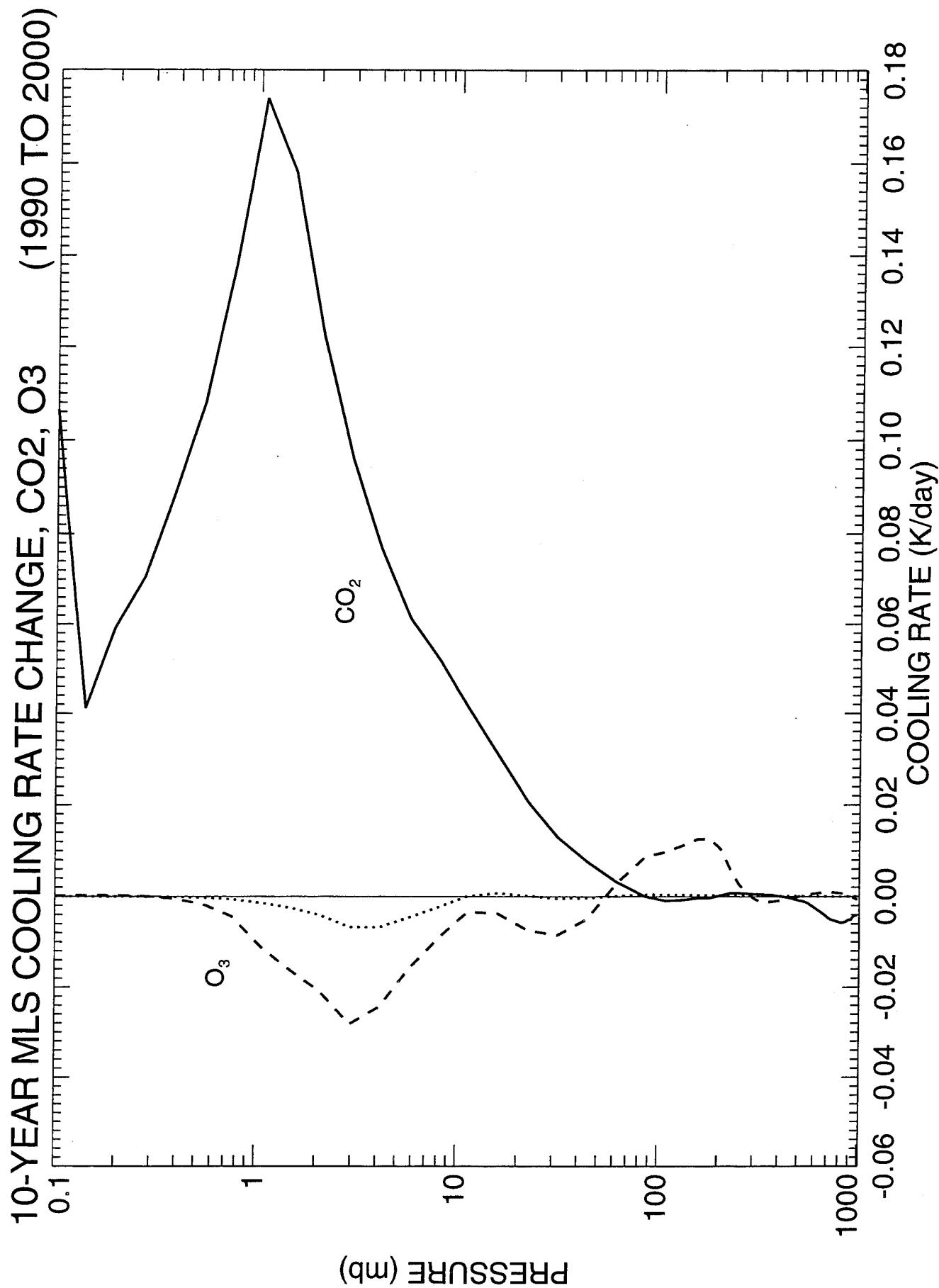


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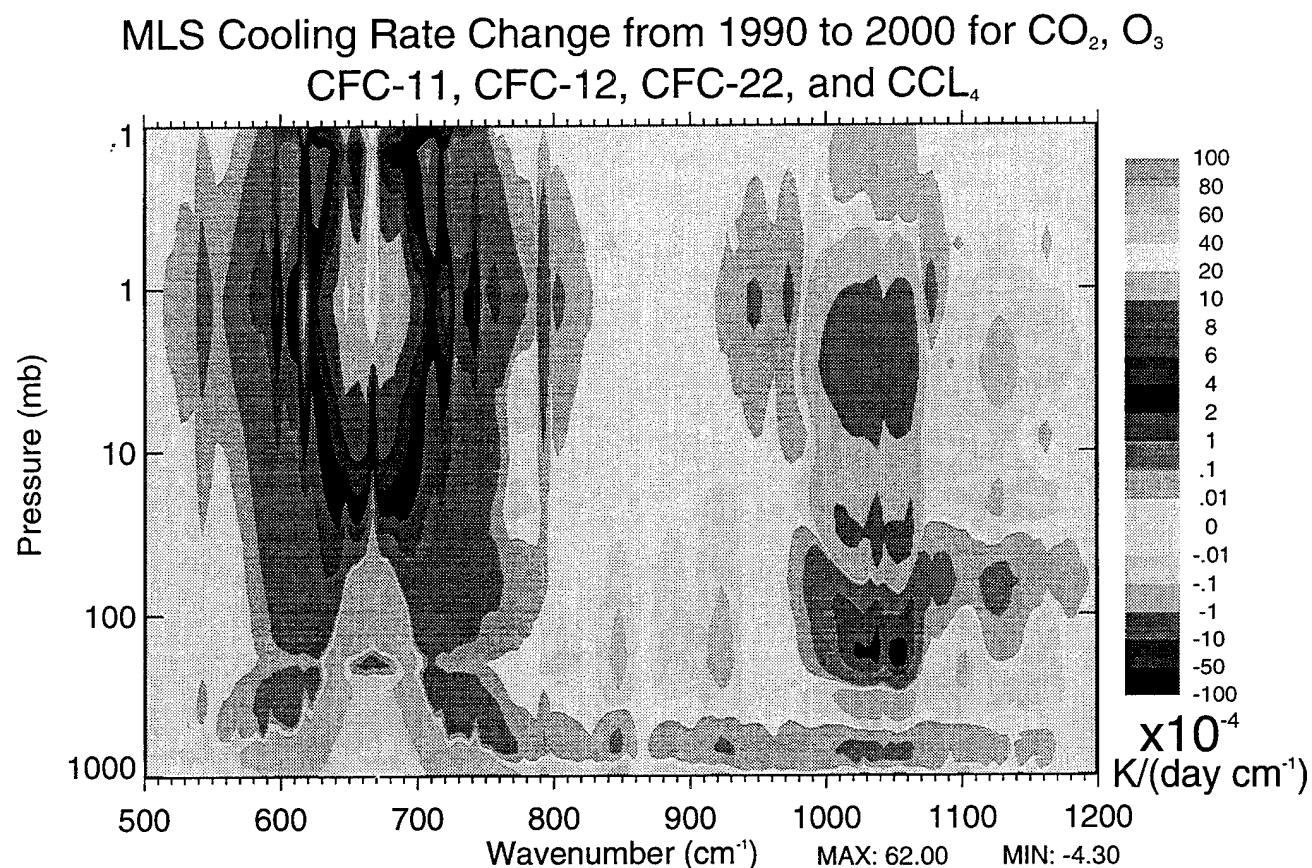


1990 TO 2000 PERCENT CHANGE IN MOLECULAR AMOUNTS, MLS

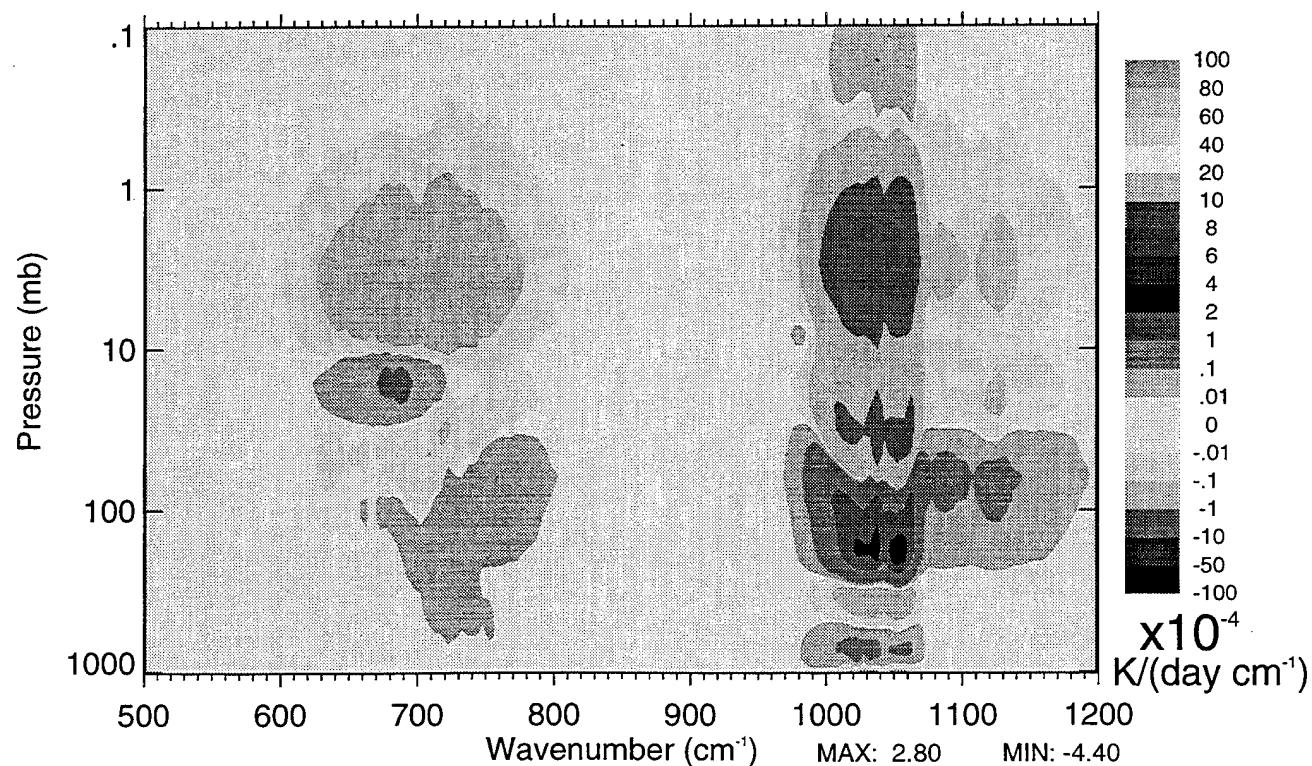




# 10-Year Changes in Cooling Rate from 1990 to 2000



MLS Cooling Rate Change from 1990 to 2000 for Ozone Only



## Conclusions

### Water Vapor:

- The dominant greenhouse gas on a global basis for the troposphere
  - For atmospheres with significant amounts of water vapor, increases in concentration of a uniformly mixed gas result in a reduction in the atmospheric cooling in the lower troposphere
- Cooling in the upper troposphere is dominated by water vapor in the pure rotation region ( $0\text{-}400\text{ cm}^{-1}$ ),

### Carbon Dioxide and Ozone:

- Strong absorbers, but only over narrow spectral regions
  - $\text{CO}_2$  eliminates cooling below 500mb due to water vapor
  - from  $640\text{-}690\text{ cm}^{-1}$
- Doubling of carbon dioxide causes decreased cooling in the lower troposphere of about 5%
- Ozone exchange heating occurs from 500 to 20 mb; peaks at 0.3 K/day at 50 mb level

### Halocarbons, $\text{CH}_4$ , and $\text{N}_2\text{O}$

- These gases diminish  $\text{H}_2\text{O}$  cooling in lower troposphere in moist atmospheres, but have little affect on cooling in dry atmospheres
- Effects on outgoing flux and surface downwelling flux are non-negligible

### 1990-2000 Changes

- Radiative effects of ozone are highly dependant on depletion profile
- Stratospheric heating effect of ozone depletion offsets about 16% of the total cooling effect of carbon dioxide at this level
- $700\text{ cm}^{-1}$  ozone band is significant; contributes a maximum of 25% of the total ozone cooling response to ozone profile perturbations

VERY NARROW BAND MODEL CALCULATIONS OF  
ATMOSPHERIC FLUXES AND COOLING RATES  
USING THE MODTRAN CODE<sup>\$</sup>

Presented By

L. S. BERNSTEIN, A. BERK, P. K. ACHARYA,  
AND D. C. ROBERTSON  
*SPECTRAL SCIENCES, INC.*

G. P. ANDERSON, J. H. CHETWYND, AND L. M. KIMBALL  
*GEOPHYSICS DIRECTORATE, PHILLIPS LABORATORY*

Presented At

ANNUAL REVIEW CONFERENCE ON ATMOSPHERIC  
TRANSMISSION MODELS

June 8, 1994

<sup>\$</sup> Funded by Phillips Laboratory, Hanscom AFB, Bedford, MA.



## PRESENTATION OVERVIEW

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- VERY NARROW BAND MODEL(VNBM),  $\Delta\omega = 1 \text{ cm}^{-1}$ ,  
YIELDS LINE-BY-LINE(LBL) QUALITY ATMOSPHERIC  
FLUX AND COOLING RATE PREDICTIONS.
  - $\approx 100$  TIMES FASTER THAN LBL
  - NOT TUNED TO LBL CALCULATIONS
  - INTEGRATED INTO MODTRAN
- MODTRAN UPGRADES FOR IMPROVED ACCURACY.
  - SUB-LAYER INTEGRATION
  - LINE-OVERLAP CORRECTION
  - 3-PARAMETER CG(GOODY) FOR O<sub>3</sub>
- DETAILED COMPARISONS TO ICRCM LBL RESULTS  
FOR H<sub>2</sub>O, CO<sub>2</sub>, AND O<sub>3</sub>.



## SUB-LAYER INTEGRATION\* APPROACH\*

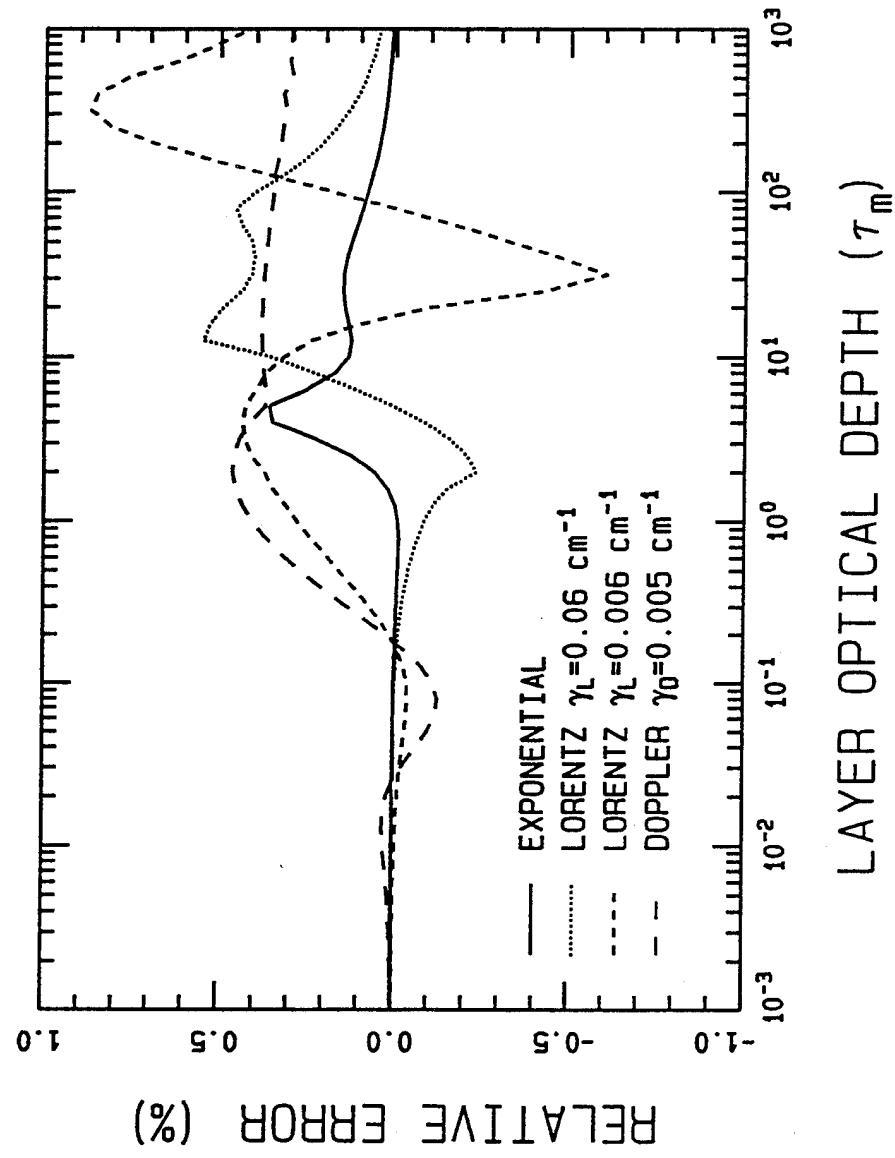
- FINE LAYERING CONVERGES SLOWLY.
- SIMPLE AND ACCURATE ANALYTICAL APPROXIMATIONS FOR BEER'S LAW ABSORPTION.
- NO SIMPLE ANALYTICAL RESULT FOR BAND MODELS.
- RATIONAL POLYNOMIAL REPRESENTATION FOR INTERVAL ABSORPTION WITH NUMERICAL INTEGRATION OF R-T EQ.
  - MOLECULAR LINE
  - 2nd ORDER PADE APPROXIMANT
  - FAST AND FLEXIBLE
  - FIVE PARAMETER FIT

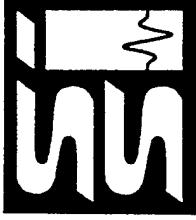
\* L. S. Bernstein, Applied Optics, Accepted, May 1994.



# SUB-LAYER INTEGRATION ERROR ESTIMATION

$\Delta\omega = 1 \text{ cm}^{-1}$  Single Line 10% Planck Function Variation

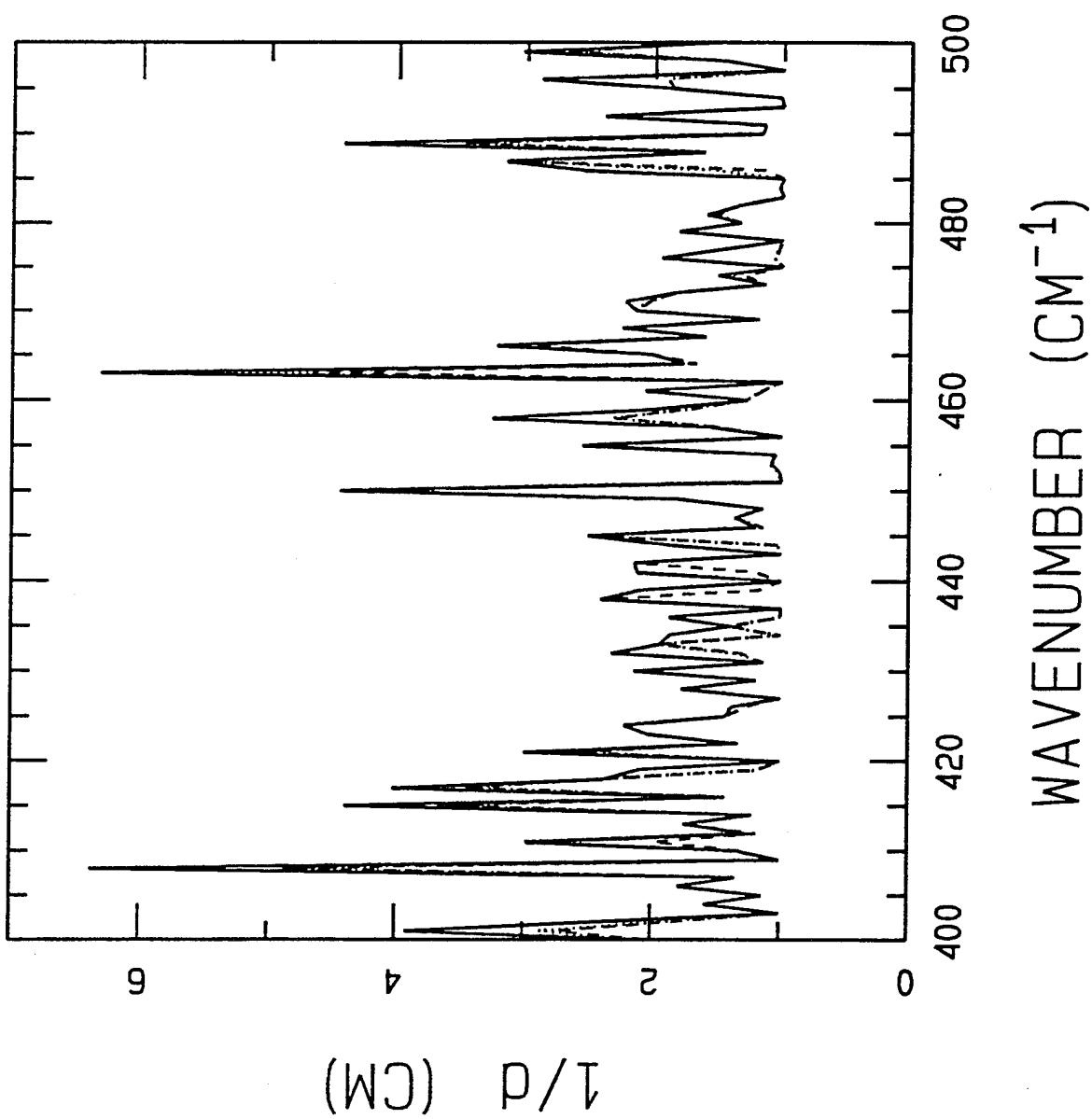




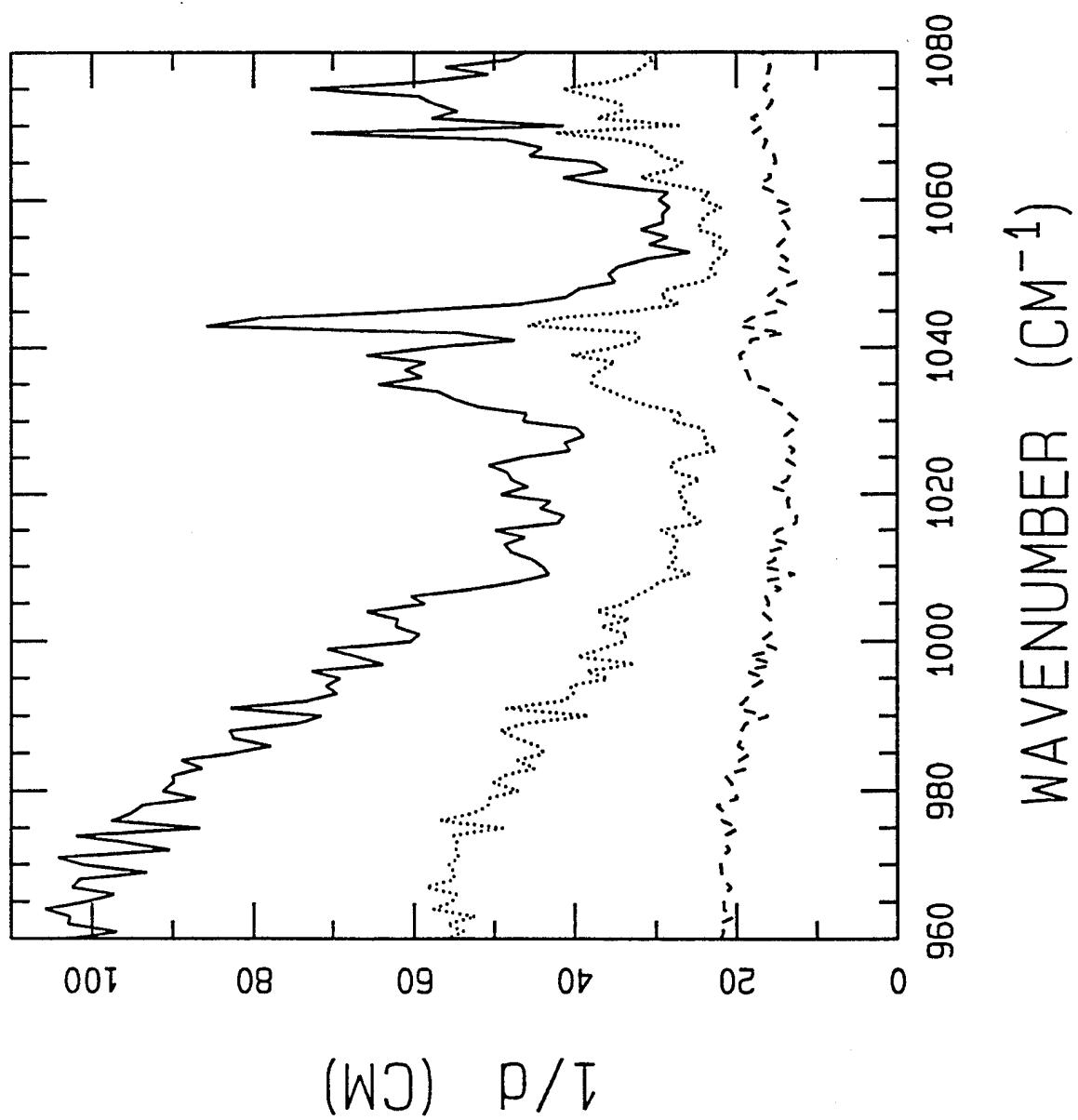
## LINE-OVERLAP CORRECTION APPROACH

- EXACT AND NEAR-EXACT LINE OVERLAPS TREATED IN COMPUTING THE LINE DENSITY PARAMETER( $1/d$ ).
  - LINES WITHIN  $\delta\omega$  COINCIDENT
  - REDUCES LINE DENSITY AND OPACITY
  - LOCAL CORRELATION APPROXIMATION(LCA)
  - $N = \Delta\omega/d$
- STATISTICAL OVERLAP CORRECTION APPLIED TO N EFFECTIVE LINES IN  $\Delta\omega$ .
  - NO POSITIONAL CORRELATION
- A SINGLE ALTITUDE AND FREQUENCY-INDEPENDENT VALUE OF  $\delta\omega = 0.01 \text{ cm}^{-1}$  WORKS WELL FOR FLUX AND COOLING RATE CALCULATIONS.

# H<sub>2</sub>O ROTATIONAL BAND



O<sub>3</sub> 9.6 $\mu\text{m}$  BAND

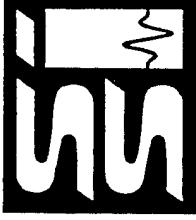




# FLUX AND COOLING RATE COMPUTATIONAL OVERVIEW\*

- 60 LAYERS.
- FLAT EARTH.
- 2 ANGLE 1st-MOMENT GAUSSIAN QUADRATURE.
- 0 - 3,000 cm<sup>-1</sup>.
- 10 AND 25 cm<sup>-1</sup> LINE TAILS.
- 27 MIN. ON HP-9000/735 WORKSTATION.  
- UNDER 10 MIN. ANTICIPATED

\* L. S. Bernstein et. al., JGR, To Be Submitted, July 1994.



## ICRCCM DATA BASE

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- ATMOSPHERIC AND ENVIRONMENT RESEARCH(AER)
  - CLOUGH ET. AL., JGR, 15, 761, 1992.
  - RES = 0.00005 cm<sup>-1</sup>
- NASA GODDARD LABORATORY FOR ATMOSPHERES(GLA)
  - RIDGWAY ET. AL., JGR, 96, 8969, 1991.
  - RES = 0.01 cm<sup>-1</sup>
- NASA GODDARD INSTITUTE FOR SPACE STUDIES(GISS)
  - LACIS AND OINAS, JGR, 96, 9027, 1991.
  - RES = 0.0005 cm<sup>-1</sup>
- NOAA GEOPHYSICAL FLUID DYNAMIC LABORATORY(GFDL)
  - SCHWARZKOPF AND FELS, JGR, 96, 9075, 1991.
  - RES = 0.005 cm<sup>-1</sup>

Table I. Summary of Line-by-Line and MODTRAN Flux Calculations.

Atmospheric Case	Flux Model	Surface (W/m <sup>2</sup> )		Tropopause <sup>(a)</sup> (W/m <sup>2</sup> )		Top (W/m <sup>2</sup> )
		UP	DOWN	UP	DOWN	
Tropical H <sub>2</sub> O with Continuum	MODTRAN	459.12	389.21	331.43	3.22	331.13
	AER	458.92	385.88	332.39	3.19	332.59
Mid-latitude Summer H <sub>2</sub> O with Continuum	MODTRAN	423.51	335.84	321.09	7.56	320.80
	AER	423.53	333.92	321.17	7.32	320.96
Subarctic Winter H <sub>2</sub> O with Continuum	MODTRAN	247.72	138.05	222.49	16.59	221.35
	AER	247.61	138.23	222.55	16.78	221.52
Mid-latitude Summer H <sub>2</sub> O without Continuum	MODTRAN	423.51	269.58	334.98	7.15	334.77
	MODTRAN <sup>(b)</sup>	423.51	269.35	335.34	6.98	335.12
	AER	423.32	269.02	335.77	6.89	335.66
	GLA	423.48	267.28	336.59	6.25	336.50
	GFDL	423.56	266.77	336.61	6.71	336.32
Mid-latitude Summer CO <sub>2</sub> (300 ppm)	MODTRAN	423.49	76.38	382.60	12.48	383.09
	GLA	423.48	76.48	383.08	12.14	383.65
	GISS <sup>(c)</sup>	422.85	76.35	382.01	12.22	382.68
	GFDL	423.56	76.28	383.26	12.15	383.72
Mid-latitude Summer CO <sub>2</sub> (600 ppm)	MODTRAN	423.49	84.40	377.67	14.23	378.99
	MODTRAN <sup>(b)</sup>	423.49	76.22	382.75	12.38	383.22
	GLA	423.48	84.66	377.95	13.91	379.37
	GLA <sup>(d)</sup>	421.29	83.70	376.67	13.89	378.03
	GFDL <sup>(d)</sup>	421.38	83.60	376.83	13.92	378.07
Subarctic Winter CO <sub>2</sub> (300 ppm)	MODTRAN	247.71	44.17	231.50	14.52	229.83
	GLA	247.71	44.22	231.64	14.15	230.17
	GFDL <sup>(d)</sup>	247.36	43.90	231.44	14.16	229.94
Mid-latitude Summer O <sub>3</sub>	MODTRAN	433.49	6.33	419.34	3.26	411.64
	MODTRAN <sup>(b)</sup>	423.49	6.16	419.40	3.06	412.11
	GLA	423.48	6.00	419.60	3.10	412.02
	GISS <sup>(c)</sup>	422.85	6.40	418.61	3.31	410.84
	GFDL	423.56	6.18	419.43	3.04	412.06

(a) 99.7 mbar (TROP), 179 mbar (MLS), 282.9 mbar (SAW).

(b)  $\delta\omega = 0.01 \text{ cm}^{-1}$  ( $\delta\omega = 0.0 \text{ cm}^{-1}$  for all other MODTRAN runs).(c) 0 - 2,500  $\text{cm}^{-1}$  spectral interval.(d) 0 - 2,200  $\text{cm}^{-1}$  spectral interval.

Fig. 1

H<sub>2</sub>O LINES AND CONTINUUM

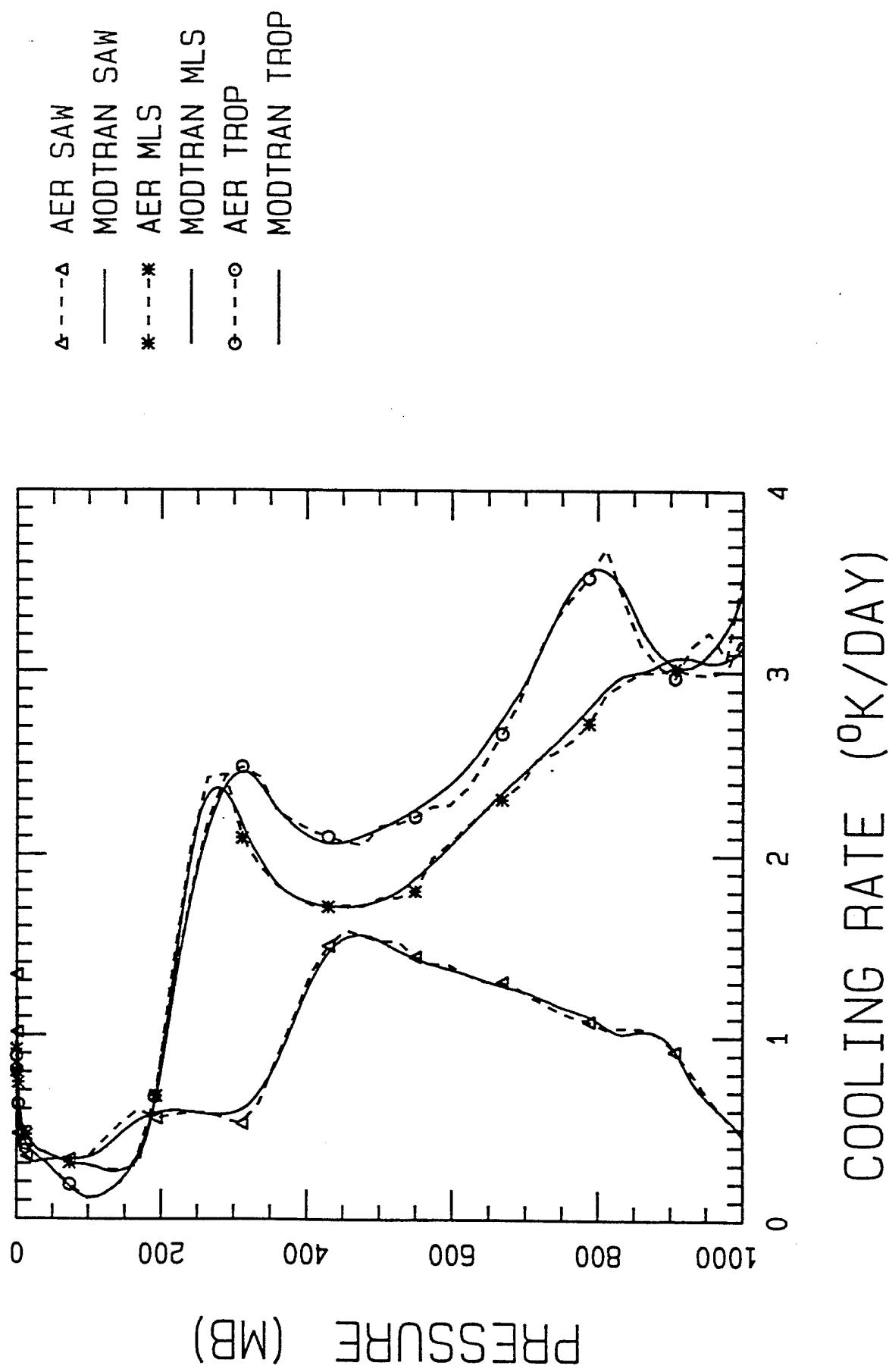


Fig. 3

H<sub>2</sub>O LINES AND CONTINUUM

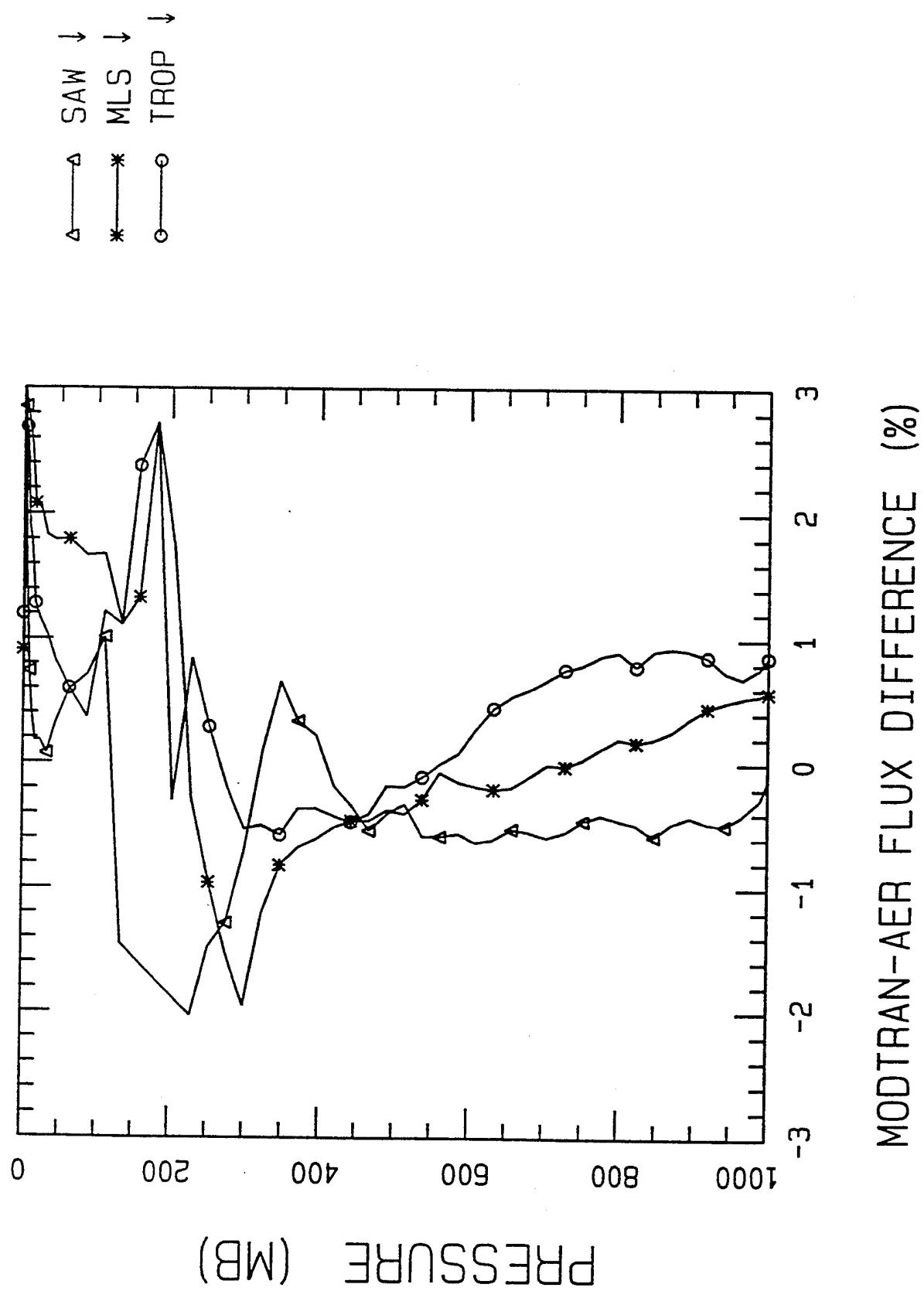


Fig. 4

H<sub>2</sub>O LINES ONLY

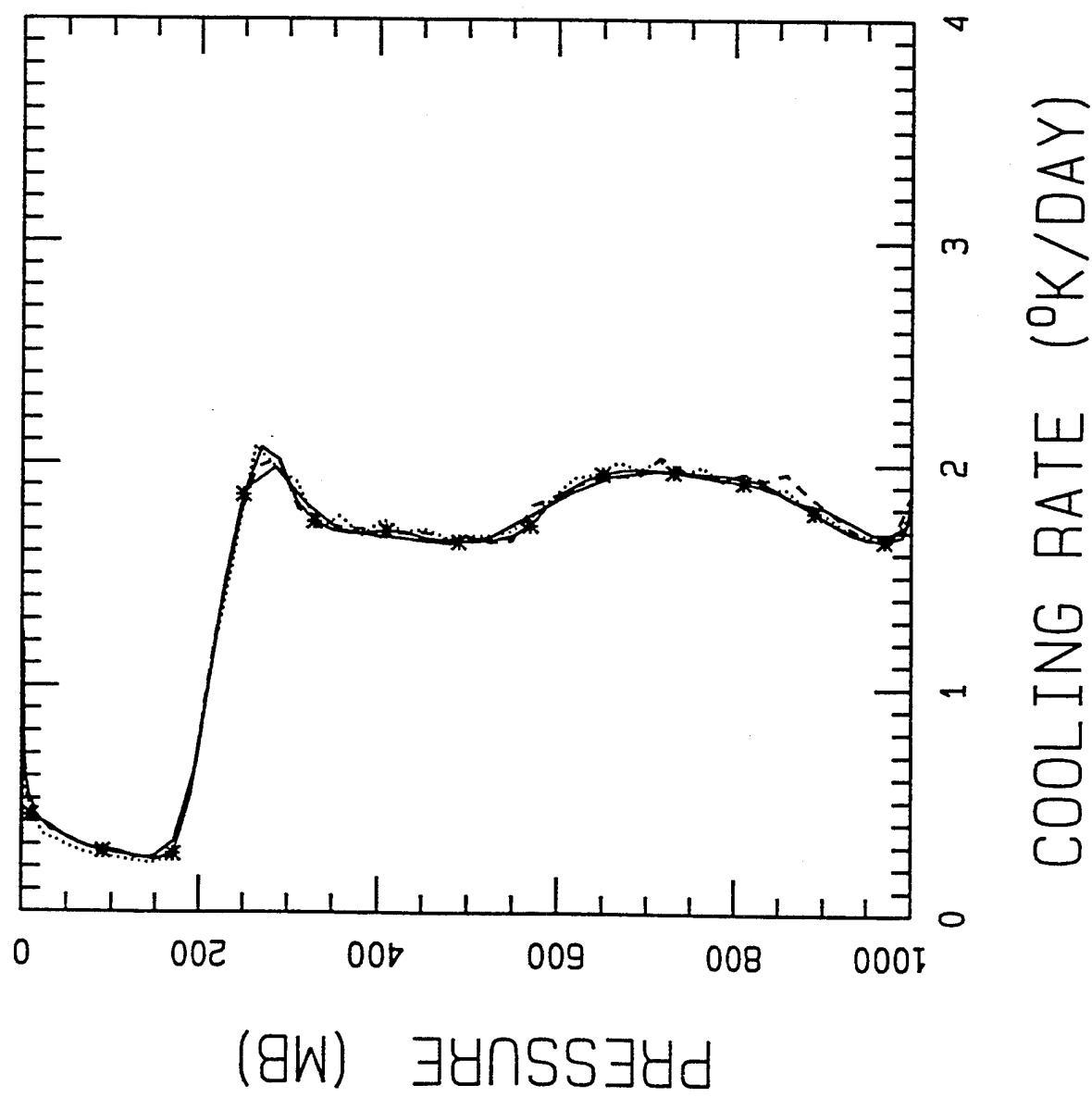


Fig. 6

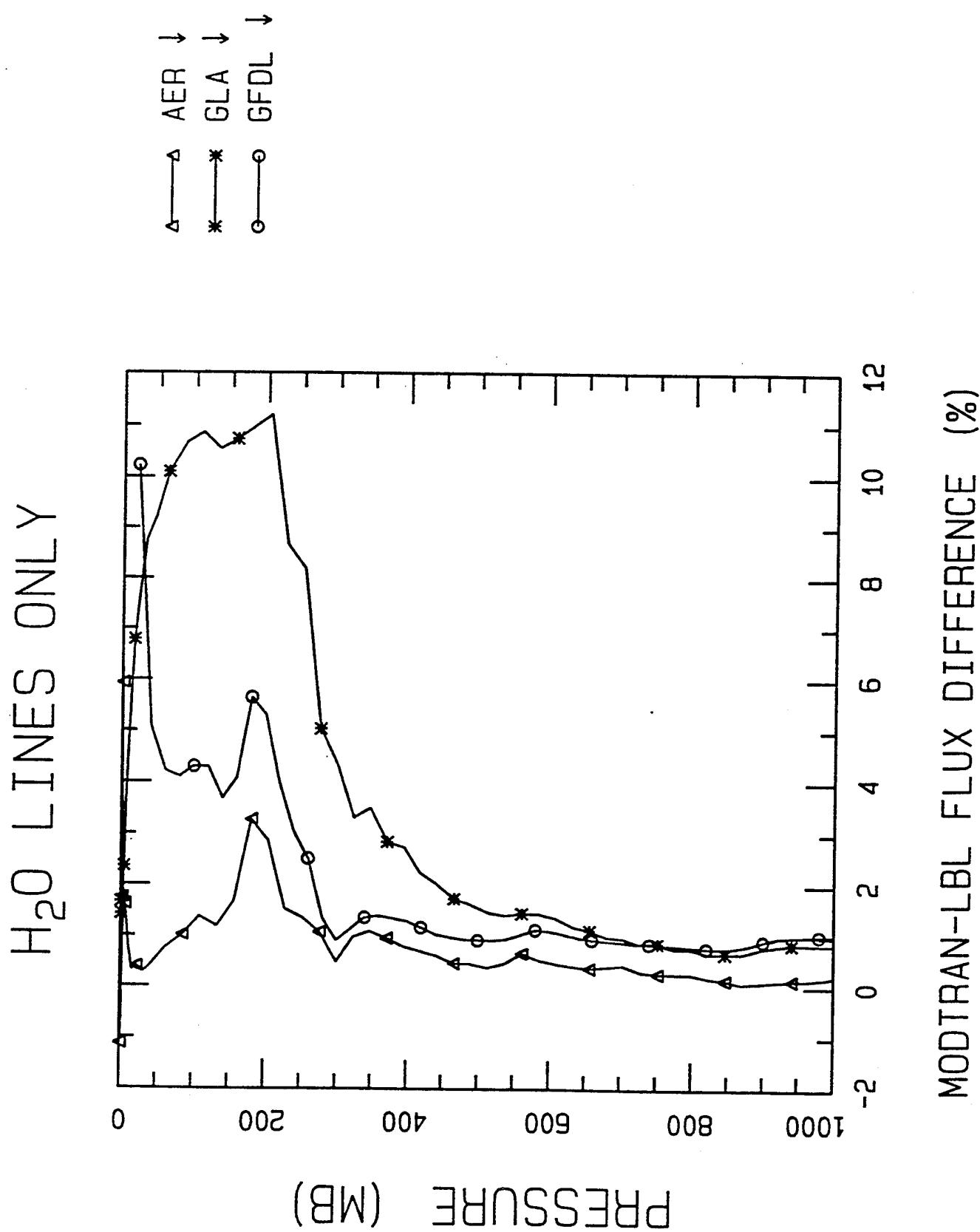


Fig. 21

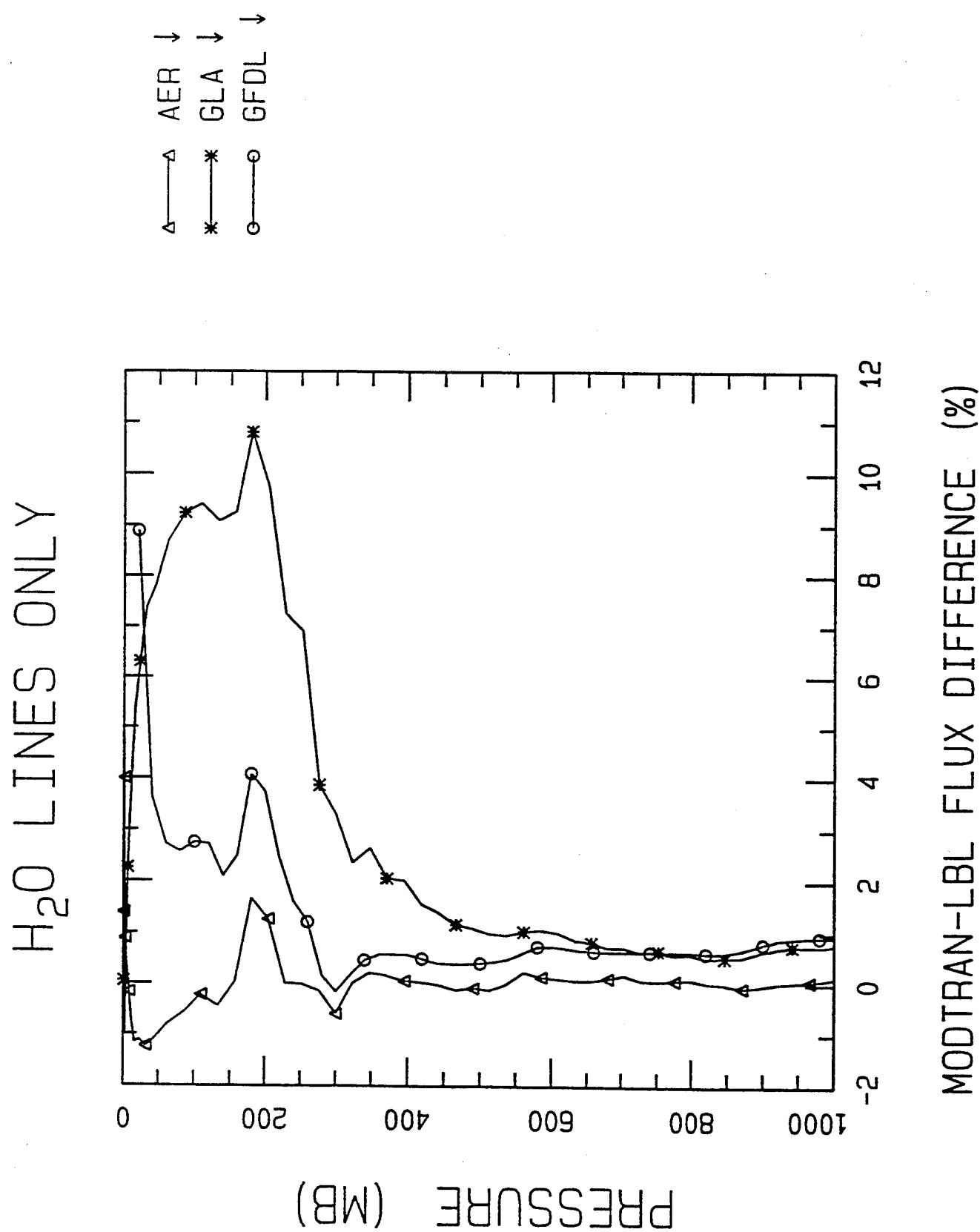


Fig. 7

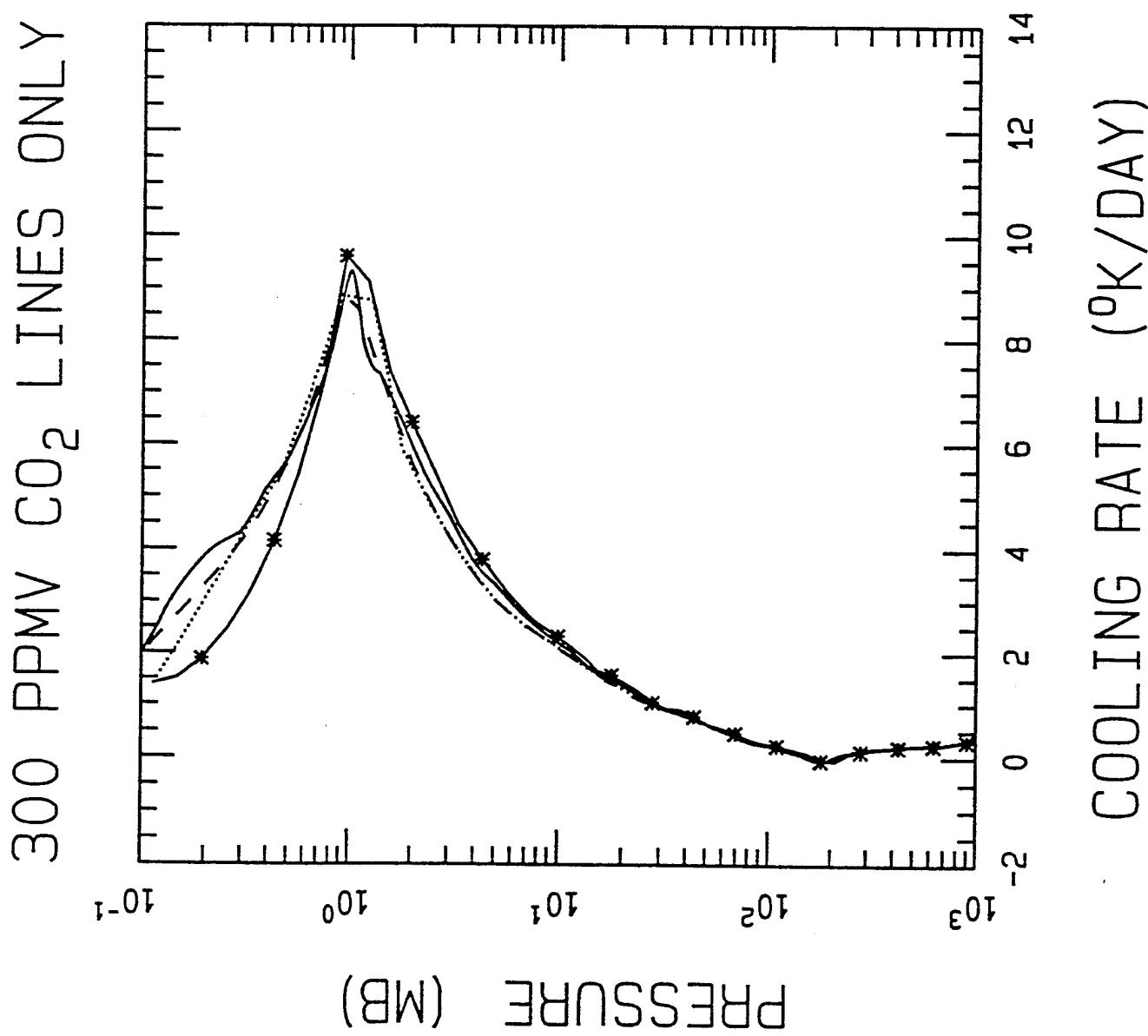


Fig. 22

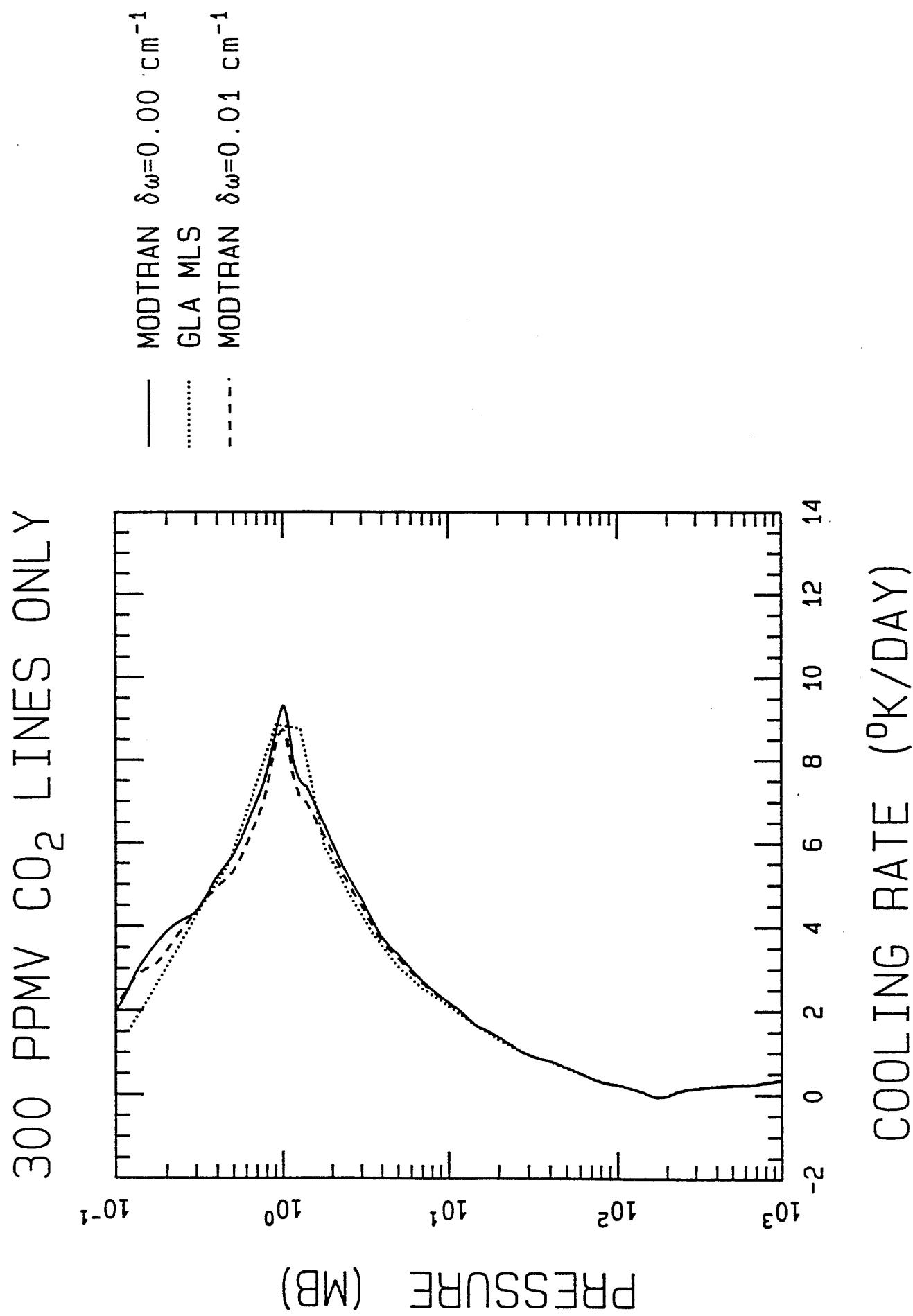


Fig. 9

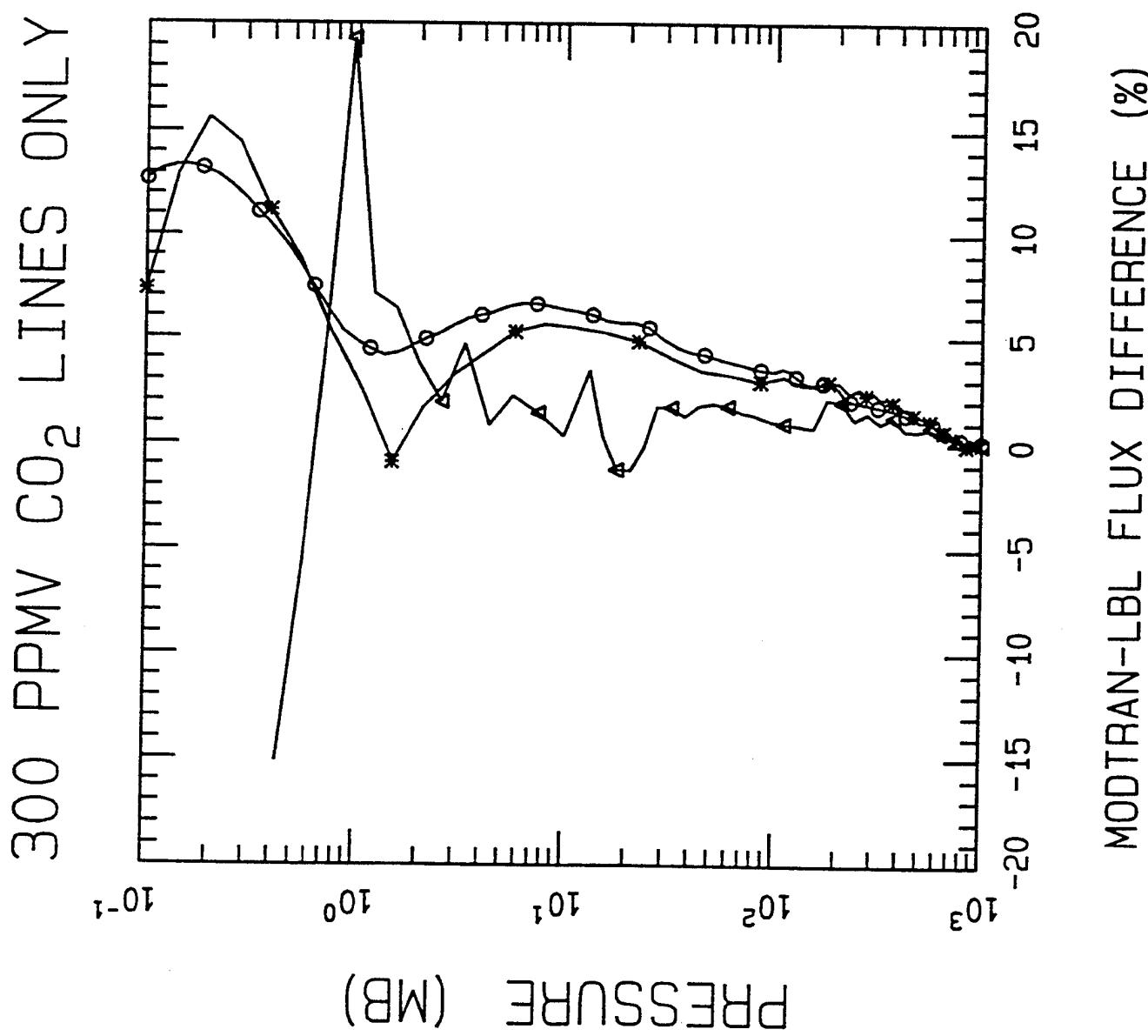


Fig. 23

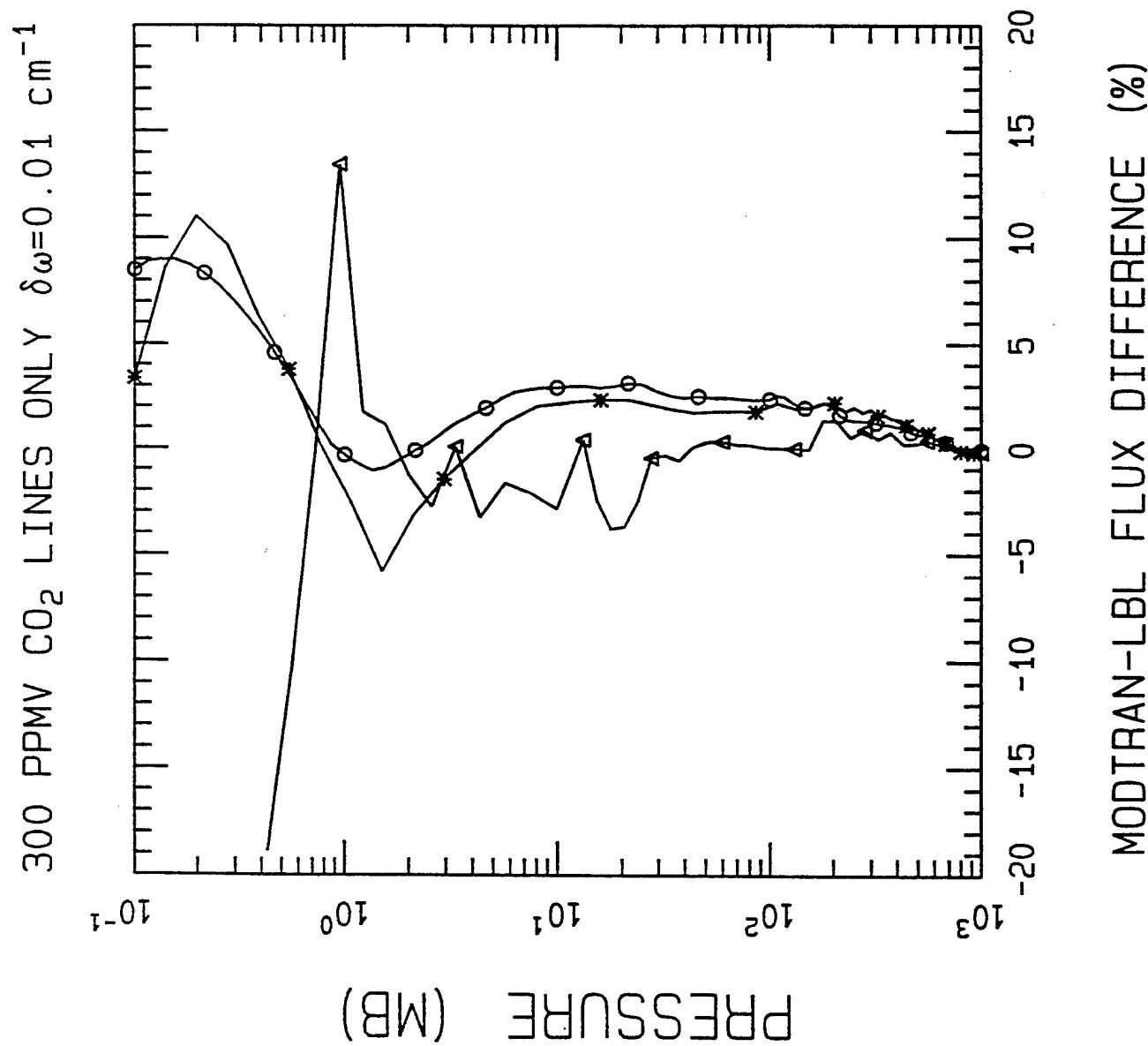


Fig. 15

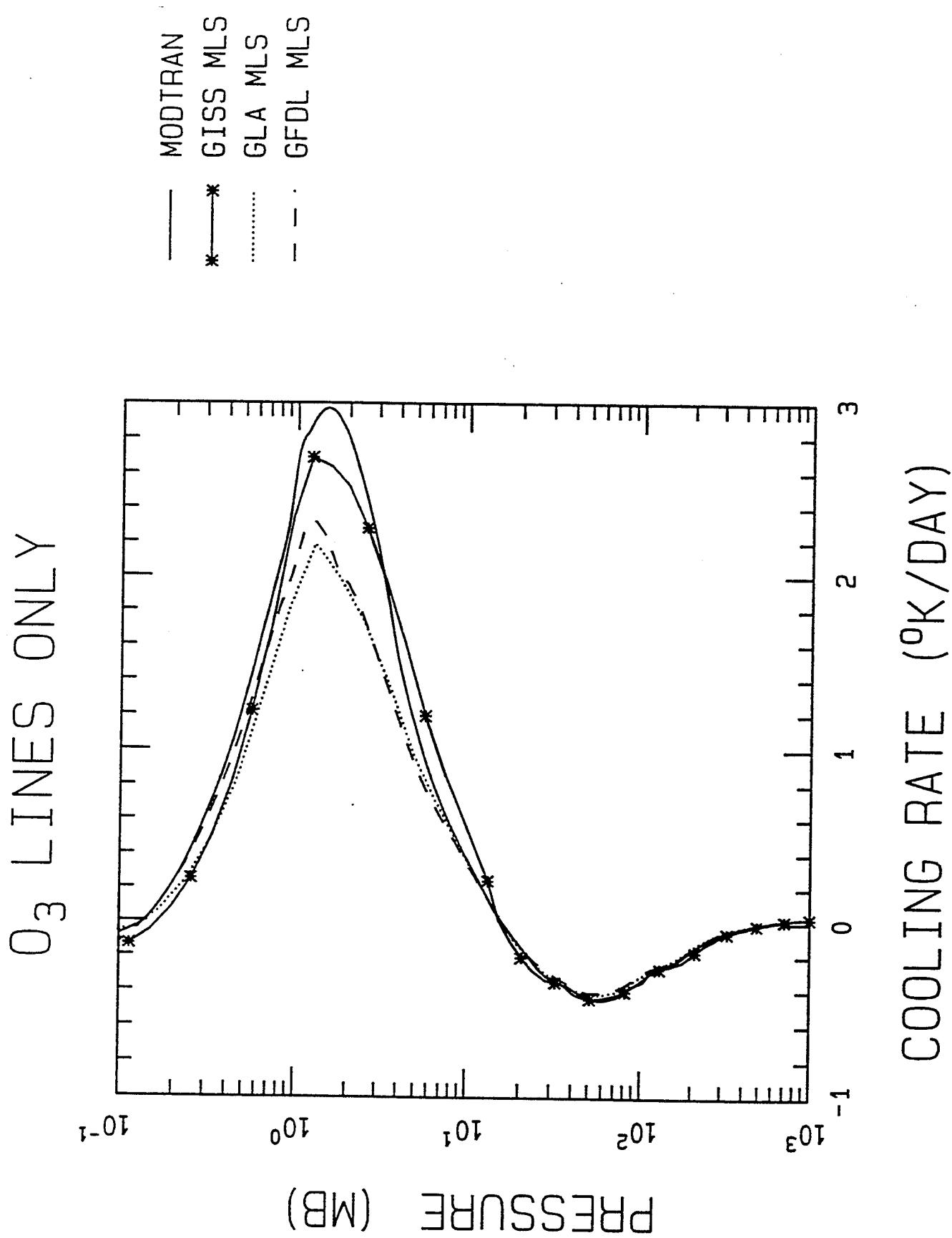


Fig. 24

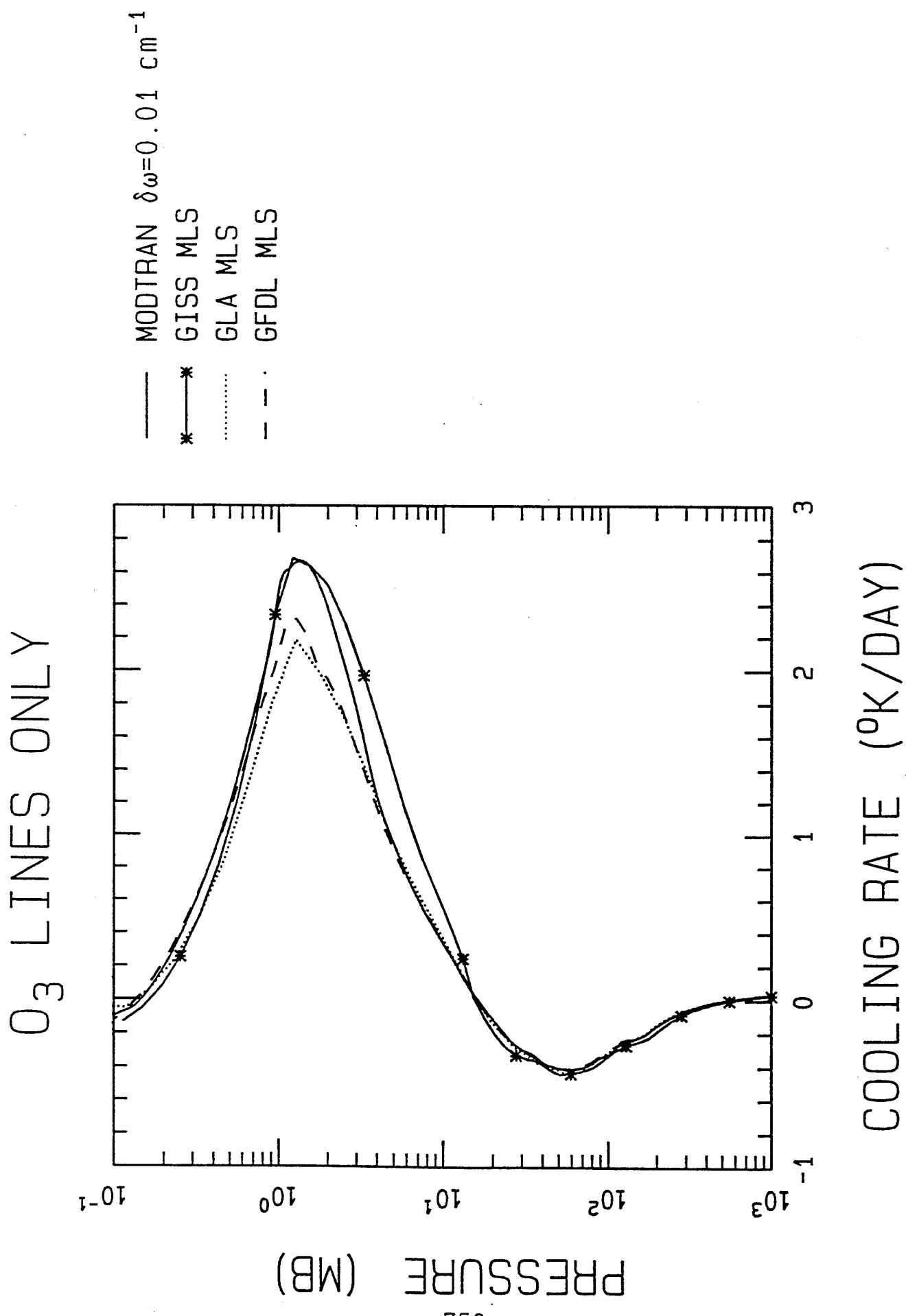


Fig. 17

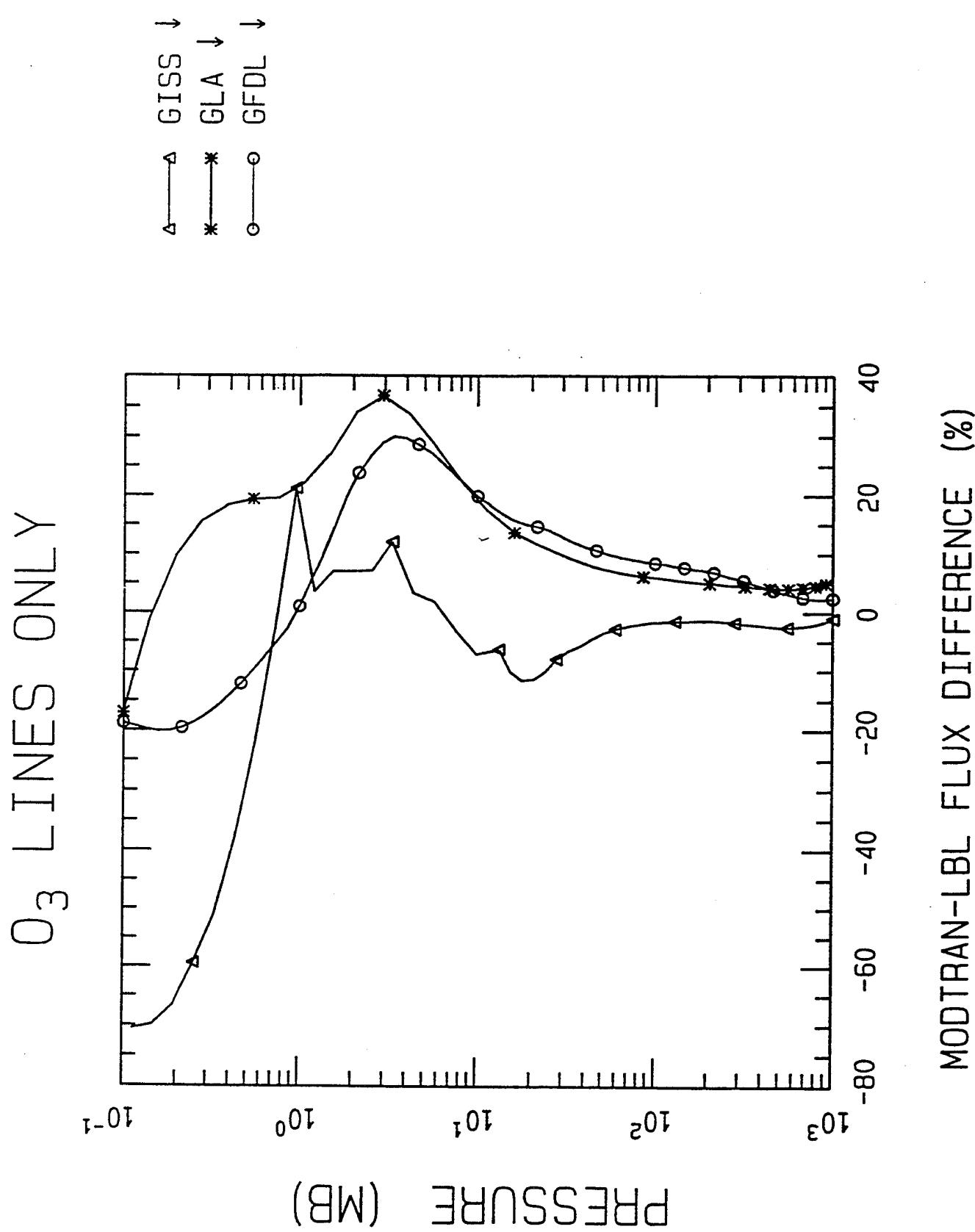
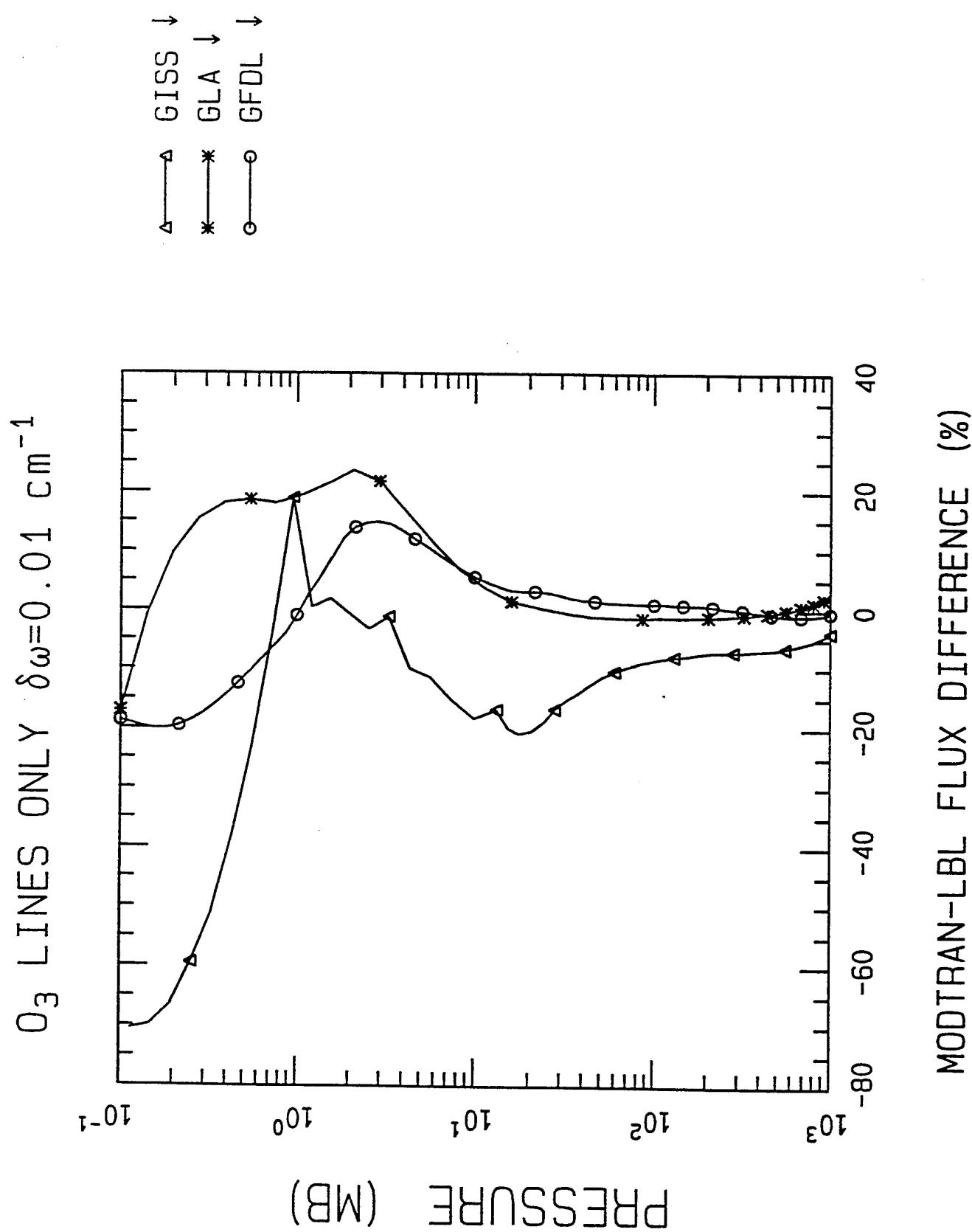


Fig. 25





## CONCLUSIONS

- $1 \text{ cm}^{-1}$  VNBM INCORPORATED INTO MODTRAN.
- MODTRAN-PREDICTED FLUXES AND COOLING RATES WITHIN SPREAD OF LBL RESULTS FOR  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ , AND  $\text{O}_3$ .
  - HIGH ALTITUDE ISSUES
- FUTURE MODTRAN DEVELOPMENTS.
  - LCA REFINEMENTS
  - SCATTERING
  - SPECTRAL RESOLUTION

## ACKNOWLEDGEMENTS

---

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APPLIED RESEARCH CORPORATION

M. J. IACONO  
ATMOSPHERIC AND ENVIRONMENTAL RESEARCH

# **Greenhouse Gas Concentration Profiles Retrieved from CIRRIS-1A Measurements in the 7-13 $\mu\text{m}$ window during STS-39**

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Geophysics Directorate, Phillips Laboratory, Hanscom Air Force Base, MA 01731

## **Abstract**

The spectral and spatial distributions of the greenhouse gas infrared emissions are measured by the CIRRIS-1A (Cryogenic Infrared Radiance Instrumentation for Shuttle) interferometer sensor during STS-39 flight (28 Apr - 6 May, 1991). The spectra in the important 7-11  $\mu\text{m}$  infrared window were recorded. High resolution spectral scans ( $\sim 1.5 \text{ cm}^{-1}$  instrument resolution) and FASCOD-3 with HITRAN92 database and NMC temperature and pressure profiles are used in an onion peel routine to retrieve gas concentrations from absolutely calibrated radiance data. Scan to scan and profile to profile variability are compared to show the measurement capability of the cryogenic infrared interferometer. The local aerosol is estimated by comparing the modelled and measured  $\text{CO}_2$  hot band (10.5  $\mu\text{m}$ ) spectra. The results of concentration profiles retrieved from the spectra (30° south latitude 9° East longitude, local time of 1.2 hr.) are shown in the figure. Profiles of CFC-11, CFC-12,  $\text{HNO}_3$ , and  $\text{O}_3$  developed in this fashion and at different locations are compared with ATMOS (Atmospheric Trace Molecule Spectroscopy), LIMS (Limb Infrared Monitor of the Stratosphere), and situ mean data for these gases.

## **Conclusion**

The infrared emissions from greenhouse gases were successfully measured as part of the STS-39 mission and the calibrated spectra used to obtain the spatial distribution of some of these gases. As an example, the vertical concentration profiles of  $\text{O}_3$ ,  $\text{HNO}_3$ , CFC-12, CFC-11, and aerosols were retrieved from one of the CIRRIS-1A measured spectral profiles collected in the southern hemisphere (30° S, 9° E). Specific errors in the retrieval routine are shown. Other data profiles are in preparation to be published separately.

The CIRRIS-1A data set demonstrates the capability of a moderate resolution interferometer to monitor global distributions of the most prominent greenhouse gases in the 7-13  $\mu\text{m}$  window. Since these gases are also active in the ozone reduction cycle, these data are doubly important. Use of the  $\text{CO}_2$  laser band at  $940 \text{ cm}^{-1}$  provides an effective way to estimate aerosol emissions in the region where these emissions segregate offset trace gas retrieval. A

major limitation of the CIRRIS-1A instrument complement, as it was flown, was the specific instrumentation with the lack of capability to measure gas temperature and pressure while simultaneously collecting spectral signatures. One of the large error sources in the retrieval may be associated with the temperature and pressure fields of the NMC model. The accuracy of the tangent height determinations associated with this type of measurement was found to be extremely critical in the accuracy of the analysis, but was controlled in the CIRRIS-1A measurements.

Scientifically, the CIRRIS-1A data set fills an important gap in the measurements between the ATMOS and UARS data sets. The CIRRIS-1A data set does not provide a comprehensive global sampling; it is significant because it was collected only a few weeks before the Pinatubo eruption. The density profiles retrieved from other trace gases and other locations measured by CIRRIS-1A have also been performed and a detailed comparison between CIRRIS-1A profiles and comparisons with other measurements are in preparation.

---

**Figure 1.** An example of greenhouse gas emission spectrum collected at 22.4 hours local time on April 29, 1991, and tangent height of 14.08 km, latitude of  $42^{\circ}$  S longitude of  $32^{\circ}$  W, by interferometer detector 5 filter 3 ( $770\text{-}2100\text{ cm}^{-1}$ ). The primary emitters are shown in this region, with indication of analysis and retrieval regions used.

**Figure 2.** The spectral distribution, collected in one stair-step mode in the wavenumber region of  $800\text{-}1100\text{ cm}^{-1}$  and spatial region of 10-55 km. The data were taken at latitude  $30^{\circ}$  S and longitude  $9^{\circ}$  E, at local time 1.2 hours on April 29, 1991. This data set was used to present the VMR profiles in Figure 9.

**Figure 3.** CFC-11, CFC-12, and  $\text{HNO}_3$  spectral overlapping are shown in the region of  $830\text{-}960\text{ cm}^{-1}$ ; the  $\text{HNO}_3$  spectral emission is taken off of CFC-11 and CFC-12 spectrum by using spectra of different tangent heights. The major radiance peaks are identified. The data were collected at 22.4 hours local time on April 29, 1991, latitude of  $42^{\circ}$  S longitude of  $32^{\circ}$  W.

**Figure 4.** CFC-12  $v_8$  Q branch at  $1161\text{ cm}^{-1}$  is obtained by subtracting two different tangent height scans;  $\text{N}_2\text{O}$  spectrum is also shown in the same manner. The data were collected at 22.4 hours local time on April 29, 1991, latitude of  $42^{\circ}$  S longitude of  $32^{\circ}$  W.

**Figure 5.** An example of comparison of CIRRIS-1A and modelled spectra in the  $\text{CO}_2$  laser band region at a tangent height of 17.93 km which is used to retrieve the aerosol extinction.

**Figure 6.** The temperature and pressure data (from NMC) plotted in (a) and (b) at same time and location of the CIRRIS-1A data collection ( $30^{\circ}$  S,  $9^{\circ}$  E). The temperature and pressure profiles show the vertical error bar of altitude, and horizontal error bar of temperature. The data points were the chosen boundaries of the onion-peel layers. (c) the retrieved aerosol extinction at  $0.55\text{ }\mu\text{m}$  is plotted as open cycles which are actual measured points. Some other measurements are reproduced for comparison.

**Figure 7.** Examples of comparison of CIRRIS-1A and modelled spectra in the (a)  $O_3$ , (b)  $HNO_3$ , (c) CFC-12, and (d) CFC-11 band regions which are used to retrieve their VMR profiles.

**Figure 8.** The comparison between measured and modelled spectra in the large spectral region of  $800-1100\text{ cm}^{-1}$  by using retrieved VMR profiles of  $O_3$ ,  $HNO_3$ , CFC-12, CFC-11, and aerosol.

**Figure 9.** The VMR profiles of (a)  $O_3$ , (b)  $HNO_3$ , (c) CFC-12, and (d) CFC-11 retrieved from  $30^\circ\text{ S}$  and  $9^\circ\text{ E}$ , Midnight April 29, 1991 data collection (plotted in Figures 2 and 8). The open triangle data points were the chosen boundaries of the onion-peel layers, and open cycles which are actual measured points with VMR error bar. Some other measurements are reproduced for comparison.

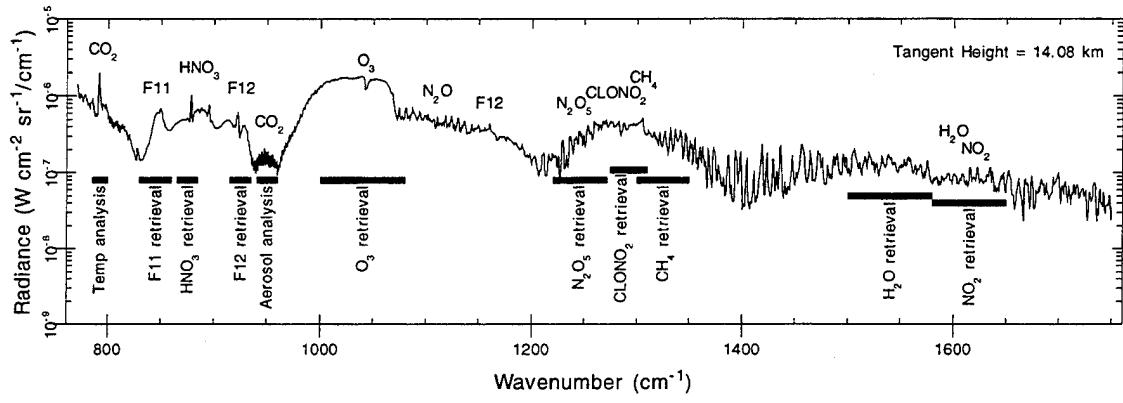


Figure 1

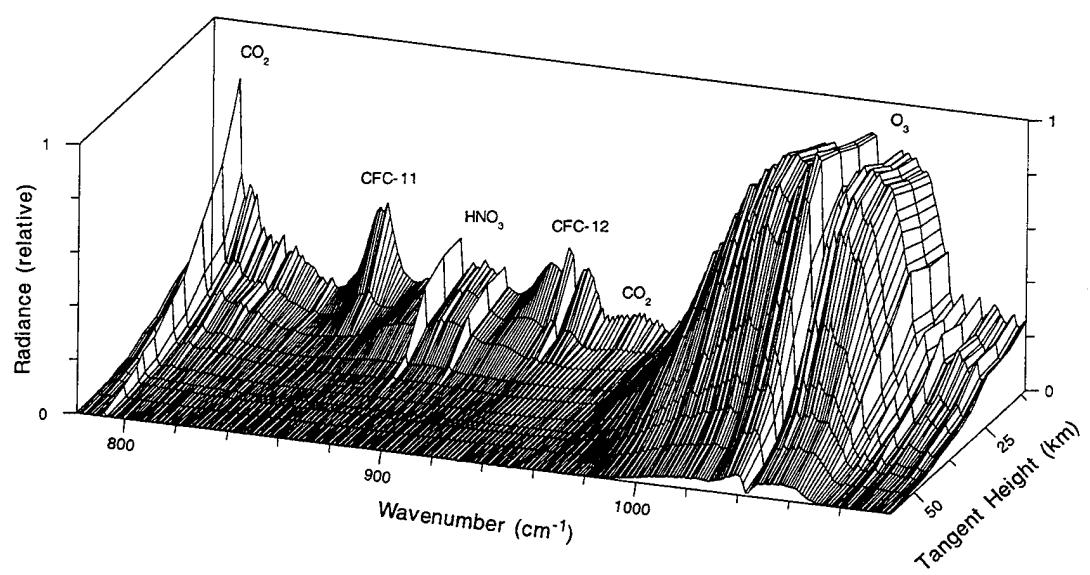


Figure 2

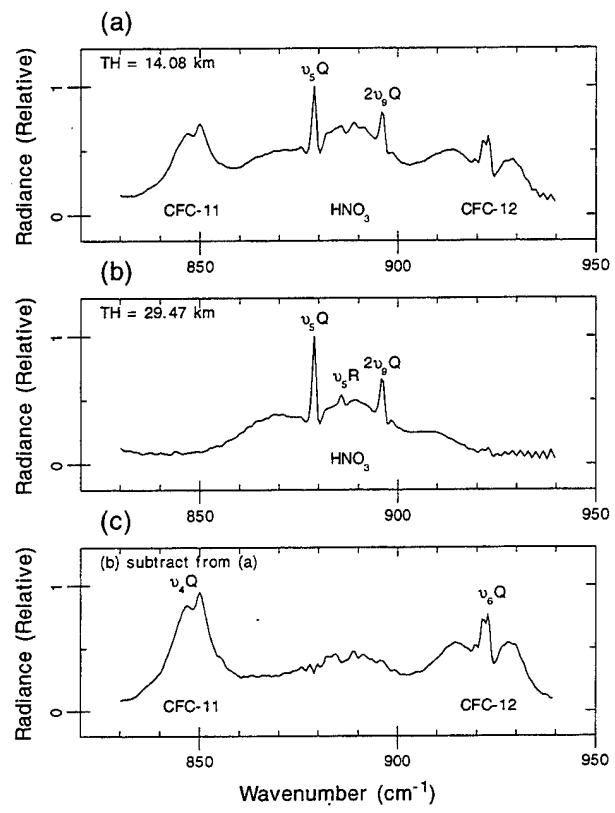


Figure 3

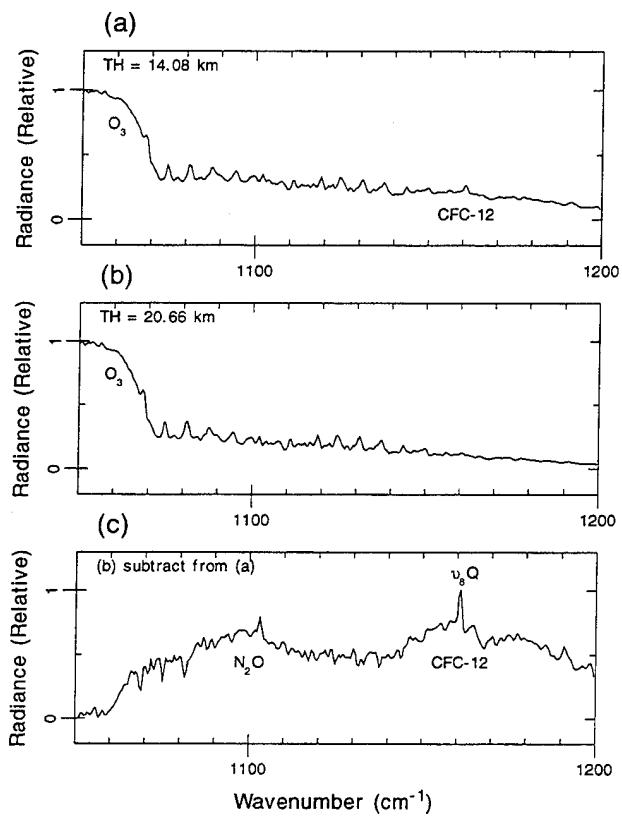


Figure 4

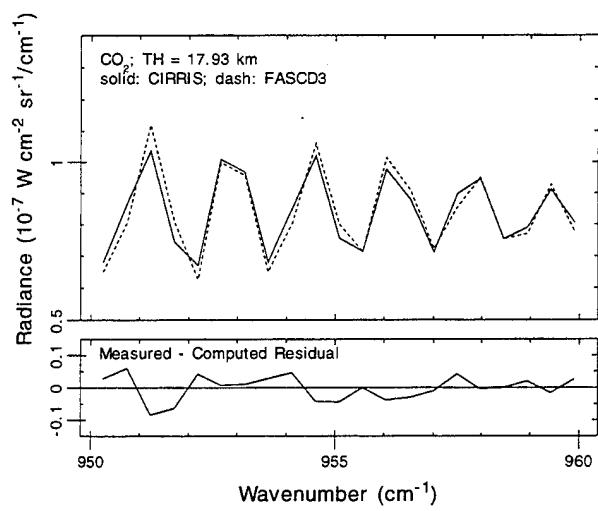


Figure 5

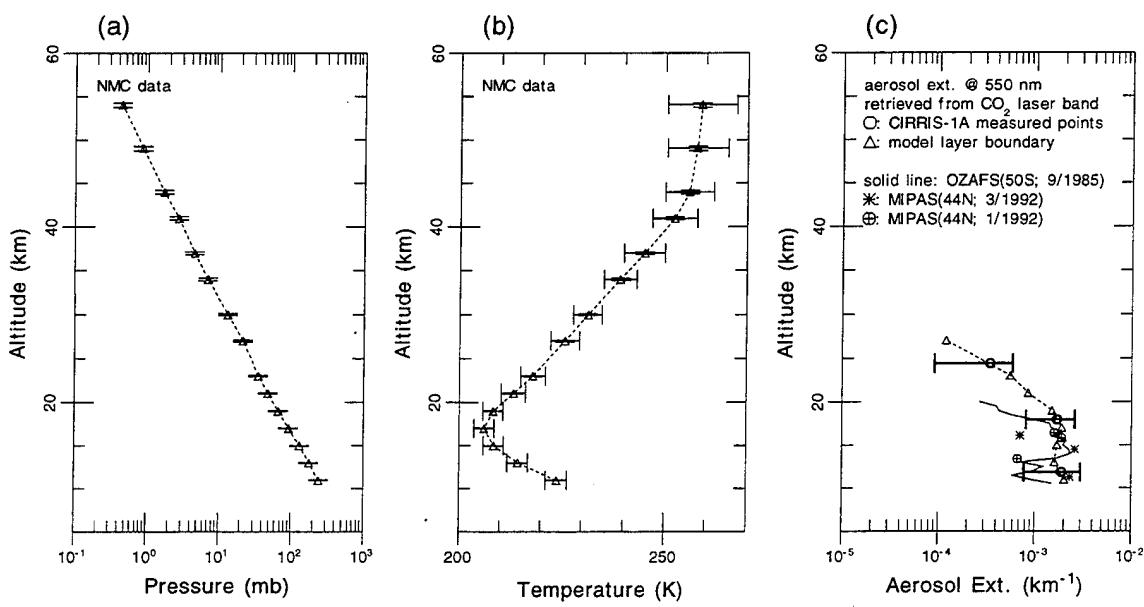


Figure 6

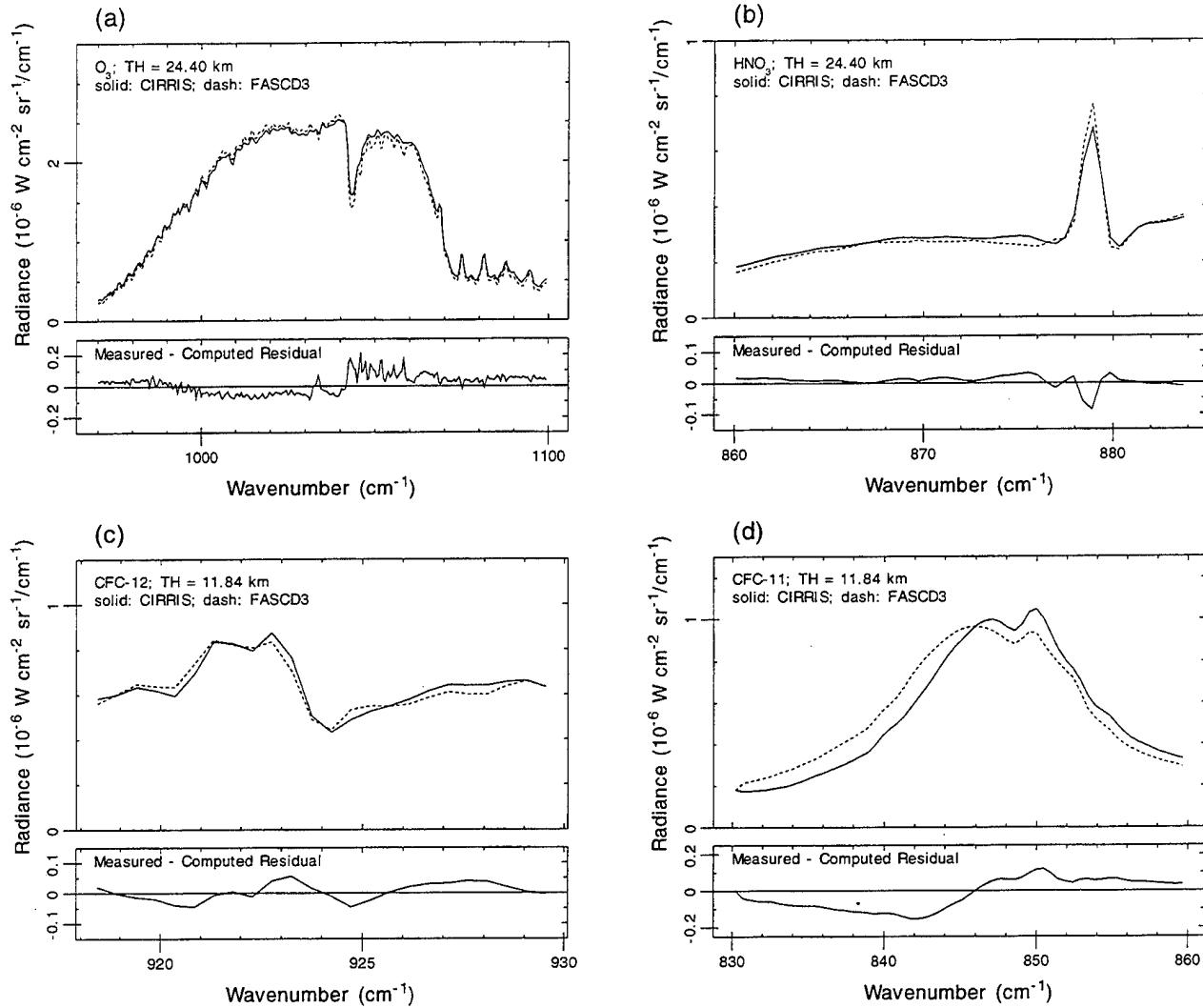


Figure 7

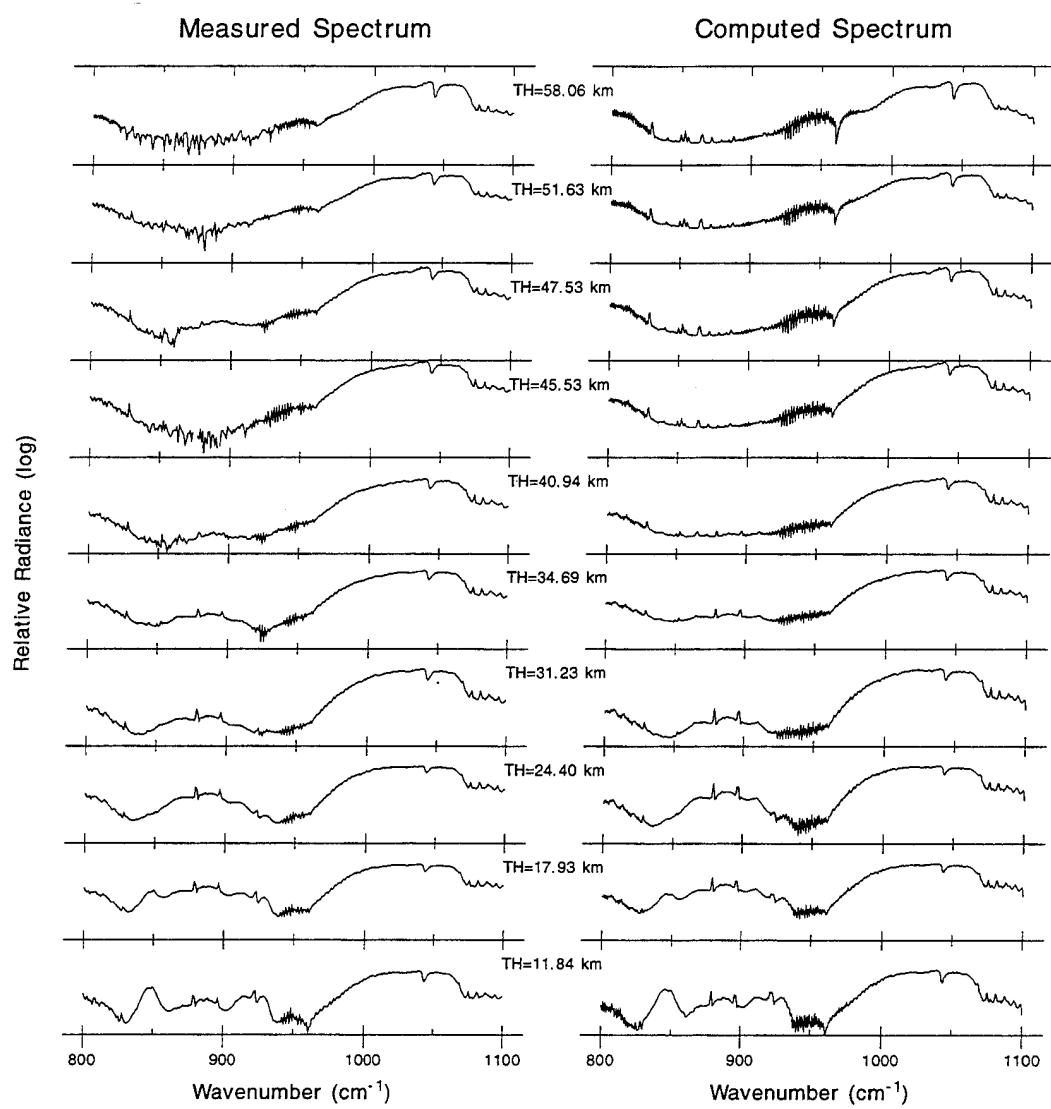


Figure 8

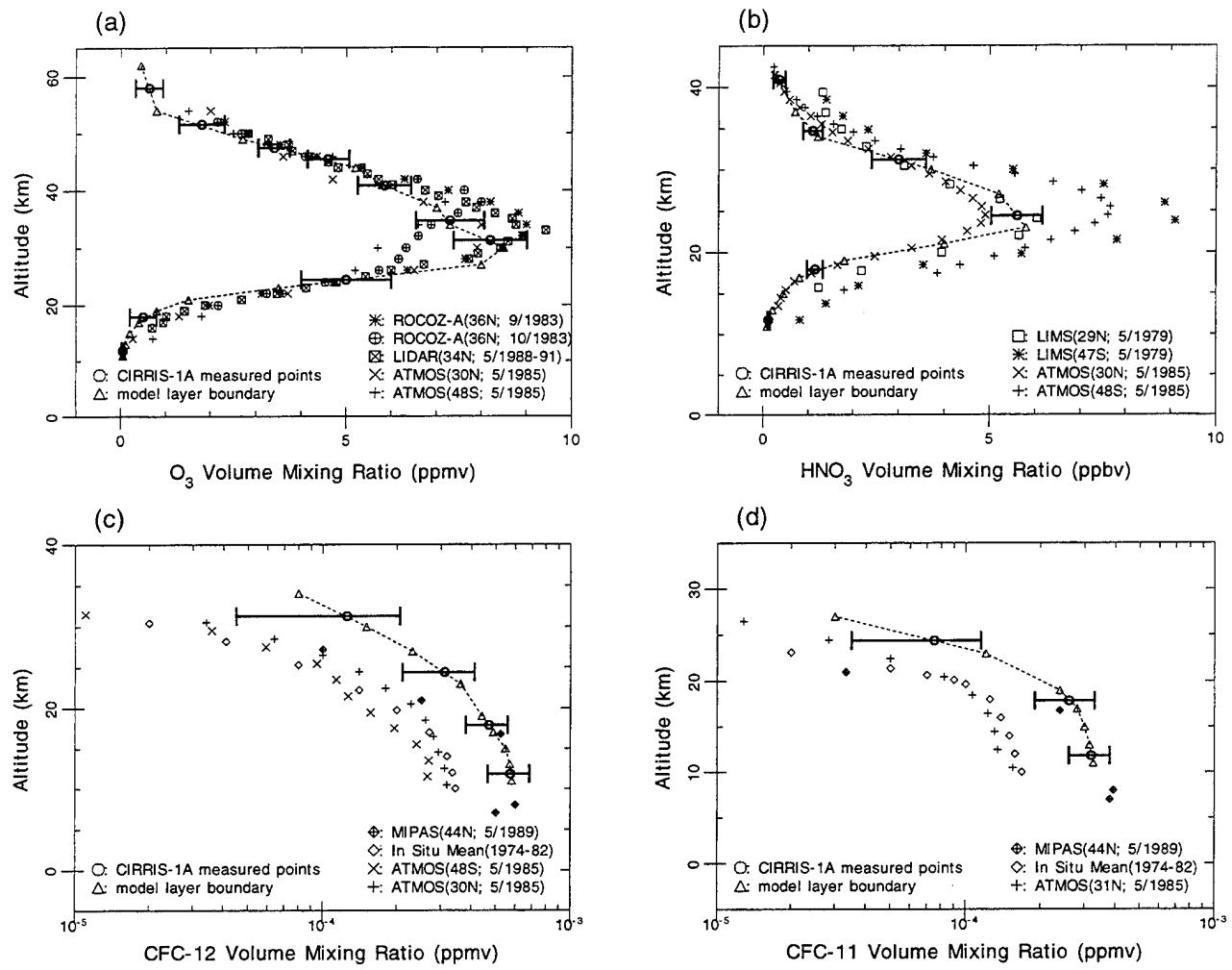


Figure 9

# **Indirect Global Warming Effects Of Ozone and Stratospheric Water Vapor Induced By Surface Methane Emission**

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*J.S. Tamarasis*

*K.O. Patten*

*A. Jain*

*K.E. Grant*

July 1994

## ***Abstract***

Methane has indirect effects on climate due to chemical interactions as well as direct radiative forcing effects as a greenhouse gas. We have calculated the indirect, time-varying tropospheric radiative forcing and GWP of O<sub>3</sub> and stratospheric H<sub>2</sub>O due to an impulse of CH<sub>4</sub>. This impulse, applied to the lowest layer of the atmosphere, is the increase of the atmospheric mass of CH<sub>4</sub> resulting from a 25 percent steady state increase in the current emissions as a function of latitude. The direct CH<sub>4</sub> radiative forcing and GWP are also calculated. The LLNL 2-D radiative-chemistry-transport model is used to evaluate the resulting changes in the O<sub>3</sub>, H<sub>2</sub>O and CH<sub>4</sub> atmospheric profiles as a function of time. A correlated k-distribution radiative transfer model is used to calculate the radiative forcing at the tropopause of the globally-averaged atmosphere profiles. The O<sub>3</sub> indirect GWPs vary from ~27 after a 20 yr integration to ~4 after 500 years, agreeing with the previous estimates to within about 10 percent. The H<sub>2</sub>O indirect GWPs vary from ~2 after a 20 yr integration to ~0.3 after 500 years, and are in close agreement with other estimates. The CH<sub>4</sub> GWPs vary from ~53 at 20 yrs to ~7 at 500 yrs. The 20 year CH<sub>4</sub> GWP is ~20% larger than previous estimates of the direct CH<sub>4</sub> GWP due to a CH<sub>4</sub> response time (~17 yrs) that is much longer than the overall lifetime (10 yrs). The increased CH<sub>4</sub> response time results from changes in the OH abundances caused by the CH<sub>4</sub> impulse. The CH<sub>4</sub> radiative forcing results are consistent with IPCC values. Estimates are made of latitude effects in the radiative forcing calculations, and UV effects on the O<sub>3</sub> radiative forcing calculations (10%).

## I. *Introduction*

The current concerns about global warming and ozone depletion have necessitated detailed studies of the potential greenhouse effects of various trace gases that have been introduced into the atmosphere. The mechanism usually used for comparison of the greenhouse potential of trace gases is the global warming potential or GWP as defined by IPCC (1990). The GWP is the ratio of the radiative flux change at the tropopause caused by the introduction of a unit mass impulse of a trace gas into the atmosphere to the radiative flux change at the tropopause caused by the introduction of a unit mass impulse of CO<sub>2</sub>. An essential part of the GWP determination is the calculation of the radiative forcing, which is defined as the radiative flux change at the tropopause produced by a unit change in the number of molecules of a particular gas with all other abundances held constant. Usually the amount of abundance change used in a radiative forcing calculation is chosen such that the change is just enough to produce a numerically significant flux change value at the tropopause. Parameterized experiments for radiative forcing have been published, for example, in IPCC (1990, 1992), and by Ramanathan et al. (1987). A model for determining GWPs has been developed by Wuebbles et al. (1992). This model approximates GWP's with an accuracy of a few percent and has been published by Wuebbles and Grossman (1992) for CF<sub>4</sub>, and Grossman and Wuebbles (1993) for SF<sub>6</sub>. In addition to the direct GWP and radiative forcing discussed above, there is the indirect GWP and radiative forcing. The indirect effects are caused when the atmospheric chemical processes produce a change in the abundance of species 2 after the introduction of an impulse of species 1. A GWP and radiative forcing effect results from the indirect abundance changes of species 2 as well as the direct GWP and forcing effect of the change in abundance of species 1. Indirect GWP effects of ozone and stratospheric water vapor have been discussed in IPCC (1990, 1992). IPCC (1990) gives an indirect ozone GWP, due to methane introduction, of 24 at a time of 20 years. IPCC (1992) gives an indirect water GWP of between 5 and 30 percent of the direct methane GWP. IPCC (1992) recommended that the indirect GWP's should be withdrawn due to incomplete understanding of the atmospheric chemical processes which cause the ozone changes. Yet, according to IPCC (1990), the indirect ozone forcing due to methane introduction could represent one of the main contributions to indirect GWP effects.

The main purpose of this paper is to reexamine the indirect effect on O<sub>3</sub> and stratospheric H<sub>2</sub>O due to a tropospheric impulse of CH<sub>4</sub> and to determine the resulting GWPs. The LLNL 2-D radiative-chemistry-transport model is used to generate a set of annually and globally averaged model atmospheres which contain the perturbed O<sub>3</sub>, H<sub>2</sub>O, and CH<sub>4</sub> abundances as a function of time. A correlated k-distribution model for the atmospheric transmission is used to calculate the tropospheric radiative forcing for CH<sub>4</sub>, O<sub>3</sub>, H<sub>2</sub>O, and CO<sub>2</sub>. These forcing values are then used to calculate the direct GWP for CH<sub>4</sub>, and the indirect GWP for O<sub>3</sub> and H<sub>2</sub>O. Estimates are made for the UV contributions to the indirect O<sub>3</sub> radiative forcing values and latitude effects on the radiative forcing calculations for O<sub>3</sub>, H<sub>2</sub>O, and CH<sub>4</sub>. Lastly, we make suggestions for future, more advanced, indirect O<sub>3</sub> and H<sub>2</sub>O, GWP calculations.

## **II. Model Atmospheres**

### **A. Model Structure**

The version of the LLNL zonally-averaged two-dimensional chemical-radiative-transport model (Kinnison et al., 1994, Patten et al., 1994, Wuebbles et al., 1991) used for these calculations determines the atmospheric distributions of 44 chemically active atmospheric trace constituents in the troposphere and stratosphere. The model domain extends from pole to pole, and from the ground to 60 km. The sine of latitude is used as the horizontal coordinate, with uneven increments corresponding to approximately 10 degrees in latitude. The vertical coordinate corresponds to the natural logarithm of pressure; the scale height is 7.2 km and the surface pressure is 1013 mb. The vertical resolution is 1.5 km in the troposphere and 3 km in the stratosphere.

### **B. Model Transport**

In the dynamics portion of the two-dimensional code, the circulation field is obtained following the approach of Garcia and Solomon (1983). Since this approach is only partially implemented in the model at the present time, we use climatological temperature and mean zonal wind fields. Both the temperature and mean zonal wind field vary continuously over the annual cycle. The temperature field is based on the reference model of Barnett and Corney (1985), while the mean zonal wind is based on data from Fleming et al. (1988). The method used to obtain the circulation is based on combining the zonal mean momentum equation and the thermodynamic equation into a form that, along with the thermal wind equation, yields a second order diagnostic equation for the residual mean meridional stream function. The net heating rate is calculated knowing the temperature and chemical species distribution and includes latent heating. The present code does not include a separate planetary or gravity wave calculation, but instead calculates the Eliassen-Palm flux directly from the zonal mean momentum equation. This is done by solving the zonal mean momentum equation.

The transport of chemical species is accomplished through both advection and turbulent eddy transport. Advection terms are treated using the second order, two dimensional transport algorithm of Smolarkiewicz (1984). The transport caused by eddy motion is parameterized through the diffusion coefficients,  $K_{yy}$  and  $K_{zz}$ . Values of  $K_{zz}$  do not vary with season, but are different between the troposphere and stratosphere. The value of  $K_{zz}$  in the troposphere is  $4 \text{ m}^2 \text{ sec}^{-1}$ , while  $K_{zz}$  in the stratosphere has values of  $0.1 \text{ m}^2 \text{ sec}^{-1}$  in the lower stratosphere increasing to  $0.25 \text{ m}^2 \text{ sec}^{-1}$  near the middle stratosphere and returning to  $0.1 \text{ m}^2 \text{ sec}^{-1}$  at the stratopause. Values of  $K_{yy}$  in the stratosphere are calculated using a similar method to that of Newman (1988) by dividing the zonal mean momentum equation (i.e., the Eliassen-Palm flux) by the horizontal gradient of the quasi-geostrophic potential vorticity. In the stratosphere, a minimum value of  $K_{yy}$  has been established as  $1 \times 10^5 \text{ m}^2 \text{ sec}^{-1}$ . The values of  $K_{yy}$  in the troposphere are assigned a value of  $2 \times 10^6 \text{ m}^2 \text{ sec}^{-1}$ . The tropopause is determined from the latitude

dependent annual mean temperature field. The height of the tropopause varies from 8 km near the poles to 14 km at the equator.

Two physical removal processes are included in the model. Surface deposition occurs in the first layer of the model. Most species are assigned a standard deposition velocity of 1 cm/sec. Nitric oxide, nitrogen dioxide, ozone, molecular hydrogen, and formaldehyde are assigned unique deposition velocities. Also, source gases emitted at the surface (e.g. methane) are assigned a deposition velocity of zero. Rainout is parameterized in the model as a first-order loss process that occurs in the first 6–7 altitude layers.

### C. Solar Radiative Transfer Model

To capture the spectral detail needed for photodissociation calculations, the two-stream multiple-layer UV-visible model uses 126 wavelength bins between 175 nm and 735 nm. The two-stream approach was chosen because of the requirements for computational efficiency placed on radiative transfer models designed for inclusion in atmospheric chemistry models. In this approach, solar radiation is effectively divided into direct solar radiation, downward diffuse radiation, and upward diffuse radiation. The scattering of energy from the direct solar beam within each individual layer is treated using the delta-Eddington algorithm (Joseph et al. 1976), which includes the dependence of scattering and absorption on the solar zenith angle. The scattering of diffuse radiation (i.e., previously scattered radiation) from each individual layer is modeled using the simpler Sagan-Pollack (1967) algorithm. Both algorithms allow inclusion of the bulk optical properties of clouds and aerosols. Finally, the adding method is used to calculate irradiances throughout the vertically inhomogeneous atmosphere.

### D. Infrared Radiative Transfer Model

The infrared model is a version of the model described by Harshvardhan et al. (1987). For our usage, it has been modified to improve the accuracy in the upper stratosphere. It includes absorption and emission by CO<sub>2</sub>, O<sub>3</sub>, and H<sub>2</sub>O. It is based on wide-band parameterizations fit to line-by-line calculations. Inhomogeneous absorption paths are included by pressure and temperature weighted scaling of trace gas absorber amounts. The model provides for specification of fractional cloud cover within each vertical model layer. Separate fractions can be specified for convective (deep, overlapping) and randomly overlapped clouds.

### E. Model Chemistry

The mechanism we are currently using in the LLNL two-dimensional model has the following characteristics:

- A total of 44 species are allowed to vary with time in the troposphere and stratosphere. Four additional species (O, O(<sup>1</sup>D), N, H) are treated as steady-state.

- There are 103 thermal (two- and three-body) reactions and 48 photolytic reactions in the mechanism.
- A complete representation of known stratospheric chemical processes.

The mechanism is listed in its entirety in Table 1. The reactions are classified by type: two-body, three-body, and photolytic. The kinetic parameters for two-body reactions are included as well.

The basic photochemistry represents the tropospheric and stratospheric interactions of actinic solar flux with the individual species in the families  $O_x$ ,  $NO_y$ ,  $ClO_y$ ,  $HO_y$ ,  $BrO_y$ , as well as with  $CH_4$  and its oxidation products. This part of the mechanism incorporates 44 transported species and 4 species for which abundance is determined through the assumption of instantaneous equilibrium. The thermal reactions considered number 103, the photolytic reactions number 48. Source gases used include  $NO_x$ ,  $N_2O$ ,  $CH_4$ ,  $CO_2$ ,  $CO$ , the chlorine compounds CFC-11, CFC-12, CFC-113, CFC-114, CFC-115, HCFC-22,  $CCl_4$ ,  $CH_3CCl_3$ ,  $CH_3Cl$ , and the bromine compounds  $CH_3Br$ ,  $CF_2ClBr$ , and  $CF_3Br$ . Most of the thermal reaction rates were taken from the NASA Panel recommendations provided in DeMore et al., (1992). The rate constant for  $CH_4 + OH$  calculated by Vaghjiani and Ravishankara (1991) was used because it represents the most recent work. Absorption cross section information has been assembled primarily from DeMore et al. (1992) and Gillotay and Simon (1991a,b). Water vapor is dealt with in a unique way compared to the other chemical species. The level of water vapor is assigned its climatological value, following the specific humidity of the Oort climatology, everywhere below the hydropause. Above the hydropause, water vapor treated as a transported species; methane oxidation is its major source in this region of the atmosphere.

The photolytic loss rate constants are calculated by integrating the product of absorption coefficient, quantum yield, and solar flux over wavelength (i.e. from 175 nm to 760 nm). The exoatmospheric solar flux is from WMO, 1985. The solar flux is then calculated as a function of altitude, latitude, and season at each time step, including the effects of absorption by  $O_2$  and  $O_3$  and multiple molecular (Rayleigh) scattering. The absorption cross sections and quantum yields include temperature and pressure dependence where appropriate and available. The Schumann-Runge band region of the  $O_2$  absorption is treated using the technique of Allen and Frederick (1982), modified to match the more recent lower cross sections of the  $O_2$  Herzberg continuum region. The photolysis of NO is also treated through the parameterization technique of Allen and Frederick (1982).

The nonlinearity of the photochemistry with respect to diurnal averaging is accounted for through the calculation of individual altitude, latitude, and seasonally varying factors for each photochemical process. Full diurnal variability of each species is calculated off-line for four seasons. The factors, relating individual process rates from the full diurnal calculation to the diurnally-averaged values, are then spline-interpolated for each time step.

Members of the ClO<sub>y</sub> family currently thought to play a role in the Antarctic spring, such as the ClO dimer, are included in this version of the model. Polar stratospheric aerosol surface has not been included. A representation of background stratospheric sulfuric acid aerosol surface is incorporated into the model, following the recommendations from the WMO, 1989 report. The reactions of N<sub>2</sub>O<sub>5</sub> and ClONO<sub>2</sub> with H<sub>2</sub>O on the aerosol surface are parameterized as first-order loss processes with rate constants determined by specified surface area density, collision frequency, and reaction probability.

#### F. Emission and Boundary Conditions

In our modeling of current and possible future atmospheres, we need to represent the surface (and atmospheric emissions) and/or surface concentrations of a number of constituents that affect tropospheric and stratospheric chemistry. A great deal of evidence indicates that surface emissions and concentrations of globally important trace gases are increasing (see WMO, 1991 for an overview). During the last ten years, scientists have been determining the atmospheric concentrations and emission rates of a variety of trace species (e.g. nitrogen oxides, carbon monoxide, and hydrocarbons) on a regional as well as global scale. These trace gases can affect the tropospheric oxidizing capacity due to changes in the levels of ozone and hydroxyl. To quantify these effects, researchers use global atmospheric models to investigate the effects of trace species. Emission inventories and measurements of the source gases are required for the initialization as well as validation of these models. The source gas fluxes must be estimated correctly in order for the models to calculate accurate species concentrations. Discrepancies between measured and calculated species concentrations can be used to check the consistency of emissions inventories, assuming all other model parameters are correct. The emphasis up to now has been to use global models to study these effects. One goal of these studies is to investigate the impact on the troposphere—ozone, hydroxyl, and oxidizing capacity.

The surface boundary conditions for the ambient version of the two-dimensional model consist of fixed concentration for nitrous oxide, molecular hydrogen, hydrochloric acid, and the halogenated organics and fluxes for methane, nitrogen dioxide, and carbon monoxide. The emission rates are specified for each latitude zone in Table 2.

Methane emissions are distributed latitudinally according to the recommendations of Fung et al., (1991). Carbon monoxide emissions are distributed latitudinally according to the emission categories defined by Hough (1991). The methane and carbon monoxide emission rates used for these calculations are obtained by determining the steady state chemical loss rate from a previous ambient model run. However, seasonal variations in the source gas emissions are not included in the results presented here. This can lead to discrepancies between the magnitudes of the calculated and observed species distributions. Another potential source of discrepancy is the representation of advective and diffusive transport in the troposphere. This would adversely affect short-lived species such as nitrogen oxides. In the current model, the diffusion coefficients are constant across all latitudes and seasons in the troposphere. We currently use diffusive transport to represent fast vertical transport processes such as convection. If the diffusivities are too

low, then species will undergo very slow vertical mixing. Fast vertical transport is often implicated in explaining unusually high levels of short-lived species in the middle and upper troposphere.

### **G. Ambient Atmosphere**

The 2-dimensional model-derived ambient atmosphere used for these calculations is based on 1990 emissions of the source gases. The two-dimensional (i.e. latitude, altitude) distributions of the radiatively important trace gases—water vapor, carbon dioxide, ozone, nitrous oxide, and methane—are averaged over the annual cycle and from pole to pole. The resulting globally- and annually-averaged altitude profiles for water vapor, ozone, and methane are depicted in Figure 1. Carbon dioxide is constant at 350 ppmv throughout the model atmosphere. Nitrous oxide decreases monotonically from 308 ppbv near the surface to 1.2 ppbv at 59 km. The pressure-temperature profile for the model atmosphere is shown in Figure 2. The tropopause in the globally-averaged atmosphere, is specified as the altitude at which the temperature gradient in the troposphere decreases to 2K/km. As indicated in Figure 2, this occurs at 166 mb (~13.2 km).

### **H. Time Dependent Atmosphere Calculations**

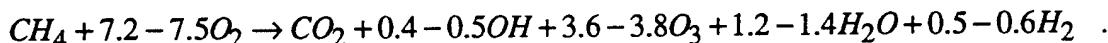
The two-dimensional model is used to determine the changes in ozone following the pulse increase in the abundance of methane. Due to its long lifetime in the troposphere, the assumed latitude and season of the methane pulse should not impact significantly the derived changes in ozone. Therefore, the pulse is distributed latitudinally at the start of the run as a percentage increase of the ambient methane concentrations. The pulse needs to be sufficiently large for the chemical model to determine an ozone change providing a significant change in radiative forcing, yet sufficiently small for the nonlinear effects on atmospheric chemistry to be minimal. Based on the analysis of ozone radiative forcing in Lacis et al. (1990), we estimate that a sufficiently large change in tropospheric average ozone concentration should be approximately 4%. This corresponds to a 25% increase of current methane emissions in our model. For the calculations in this paper we estimate the equilibrium change in the total atmospheric mass of methane for a 25% emission increase based on model results for several increased flux scenarios. The difference between the perturbed and ambient burdens, 1702.9 teragrams, is added to the surface layer in the model. We then run the model for thirty years using ambient CH<sub>4</sub> emission fluxes and initial concentrations for the other species.

Figure 3 shows the integrated change in the mass of methane calculated in the model as a function of time before and after the initial pulse as well as the ambient value of the methane mass. The methane pulse decays approximately, exponentially in time with a lifetime of the order of 17 years. The decay function with time indicates that significant nonlinear feedbacks with hydroxyl have occurred. The methane depletion rate is proportional to both the concentration of methane as well as the concentration of hydroxyl. Since the hydroxyl lifetime is of the order of five minutes, it can be assumed that the hydroxyl concentration is in equilibrium. The equilibrium hydroxyl concentration is an inverse function of the methane concentration,

$$d[CH_4]/dt = -k_1[CH_4]/(k_2 + k_3[CH_4]) + S_0 \quad , \quad (1)$$

where  $S_0$  is the background methane flux input into the atmosphere, and  $[CH_4]$  is the concentration of methane. The value of  $[CH_4]$  is the sum of the background atmosphere methane plus the extra methane due to the pulse. Eventually the methane added in the pulse will decay back to the background atmosphere methane abundance. Equation 1 implies that the methane pulse decay will be a complex function of the instantaneous methane abundance, but it will closely approximate an exponential decay with a lifetime of the order of 17 years. While the instantaneous methane lifetime in the ambient atmosphere is 10–12 years, the conjecture made in IPCC (1990) that a methane pulse will decay exponentially with a 10 year lifetime will not be the case for real methane pulses. Other analyses (Fisher, 1993, Prather, 1993) have determined that an equivalent lifetime of the order of 17 years appropriately describes the lifetime of a methane pulse in the atmosphere. We emphasize the point here that we do not use an exponential decay function in this paper, we use a direct integration of the actual radiative forcing which contains the actual value of the methane abundance at any particular time. Since the IPCC (1990) GWP numbers were based on an exponential methane decay function with a 10 year lifetime, we expect differences in the GWP values. This will be discussed in Section V. below.

Figure 4 depicts the annually-averaged change, with time, of the total ozone column calculated after the methane pulse. Figure 5 shows the calculated change with time of the annually-averaged tropospheric ozone column. Ambient values of the total and tropospheric values of the ozone column are shown in Figures 4 and 5. Total global ozone takes about six years before reaching the maximum effect while the troposphere responds within two years. The change in the ozone column abundance is a result of methane oxidation. In tropospheric regions characterized by high nitric oxide concentrations, the net methane oxidation reaction is (cf. Wuebbles and Tamarasis, 1993):



We see that complete methane oxidation results in net production of ozone. The difference in response times between the troposphere and stratosphere is due to transport, particularly across the tropopause. Since the pulse is emitted in the surface zone, dynamical processes will transport the methane upwards. Typically, it takes a long-lived gas emitted at the surface about four years to mix into the stratosphere. Furthermore, we observe that the tropospheric ozone column peaks two years after the pulse. Thus if the time constant for chemistry (two years) is added to that for transport (four years), we estimate that it should take six years for the stratospheric ozone column to peak.

Figure 6 shows the time variation of the increase in the annually and globally averaged stratospheric water vapor burden (kg). The peak value of the  $H_2O$  change occurs at a time of 10–11 years after the methane pulse. According to Lelieveld et al. (1993) the  $H_2O$  levels in the lower stratosphere are largely dependent on transport of  $CH_4$  and  $O_3$  from the troposphere. Since the stratospheric ozone peaks approximately 6 years

after the methane we expect the stratospheric water vapor to take at least this amount of time and possibly more to reach its peak value.

It is also important to consider the uncertainties in these calculations that may result both from the using a two-dimensional model in the analysis of tropospheric (and stratospheric) chemistry effects and from uncertainties in the chemistry itself. We are not able to define precisely the limits on the uncertainties at this time; however, we provide a range as a representation of overall uncertainties.

One major uncertainty is in the amount of production of ozone, in the troposphere, per unit oxidation of methane. This uncertainty depends on the reaction of  $\text{CH}_3\text{O}_2 + \text{NO}$  to produce  $\text{NO}_2$  which then photolyzes (in the troposphere) and produces ozone. The primary uncertainty in the rate of ozone formation will then largely depend on the amount of  $\text{NO}_x$  in the troposphere (we argue that the well-recognized nonlinear relationship between  $\text{NO}_x$  and ozone is unimportant to the effect of methane oxidation to produce ozone, as the production of ozone depends only on the NO conversion reaction given above). Unfortunately, tropospheric  $\text{NO}_x$  concentrations are poorly characterized globally. The two-dimensional model gives a range in the tropospheric concentrations of  $\text{NO}_x$  of 1.8–416 pptv. By comparison, the MLOPEX study (Mauna Loa Observatory Photochemistry Experiment) over the Pacific Ocean found a range of 2.4–358 pptv (Carroll et al., 1992). Measurements over polluted areas can be much larger, giving  $\text{NO}_x$  levels  $\geq 1$  ppbv. Therefore, the model appears to represent the expected values in the clean troposphere reasonably well, but may greatly underestimate the values in polluted areas. The impact of these polluted areas on the derived effects of methane will not be known until we are able to better characterize the global amounts of  $\text{NO}_x$ . Most of the uncertainty in the model representation of  $\text{NO}_x$  should be in underestimating the effects of polluted areas, but this will also depend on how well the model represents the variability of  $\text{NO}_x$  in less polluted areas of the troposphere. At this time, we believe that we can safely assume that the total uncertainty is no more than a factor of two.

### **III. Radiative Forcing Models**

#### **A. Infrared Radiative Transfer Model**

We have used an infrared radiative transfer model based on the correlated k-distribution algorithm (Grant et. al., 1992, Grossman and Grant, 1992) to calculate the radiative forcing at the tropopause. Calculations were done for a globally averaged atmosphere for  $\text{CH}_4$  and  $\text{O}_3$  at times between 1 and 30 years after a  $\text{CH}_4$  impulse has been applied at the bottom of the atmosphere. Calculations have been made of the radiative forcing for  $\text{CO}_2$ , in the globally-averaged atmosphere and at five different latitudes, 2 years after the pulse. This was done in order to determine the scaling factor with respect to the IPCC (1990) expression for  $\text{CO}_2$  radiative forcing at the tropopause. Calculations have also been made at five different latitudes for  $\text{CH}_4$  and  $\text{O}_3$ , at a time of 2 years, in order to determine the differences between the radiative forcing in the globally-averaged atmosphere and latitude averaged radiative forcing. The tropospheric radiative forcing of  $\text{H}_2\text{O}$ , caused by the methane pulse, has been calculated at five different

latitudes for times of 5, 10, 15, and 20 years after pulse. An appropriate latitudinal average is calculated to determine the globally-averaged tropospheric radiative forcing. The parameters of the calculations are;

$O_3$ ,  $CH_4$ , wave number range of 900–1650  $cm^{-1}$ , 25  $cm^{-1}$  subintervals,

$CO_2$ , wave number range of 550–1200, 2000–2525  $cm^{-1}$ , 25  $cm^{-1}$  subintervals,

$H_2O$ , wave number range of 25–3000  $cm^{-1}$ , 25  $cm^{-1}$  subintervals,

Tropopause of globally averaged atmosphere at 166 mb,

Ground Temperature of 291K (Peixoto and Oort, 1992).

The radiative forcing is defined as the difference between the net infrared flux at the tropopause in the ambient, globally averaged atmosphere, and the net flux at the tropopause in the atmosphere with changed  $CH_4$ ,  $H_2O$ , and  $O_3$  profiles calculated at the various times after the  $CH_4$  impulse.

A test of the ability of correlated k-distribution model to calculate  $O_3$  tropospheric forcing was performed using an LLNL generated model for an annually-averaged, mid latitude, clear sky atmosphere. A perturbation of 15% of the tropospheric  $O_3$  was added and the tropospheric forcing calculated. The result of 0.266  $W/m^2$  agreed to within about 10 percent of the Ramanathan et al. (1987) value for a similar test case, assuming a 20 percent correction factor for clouds. A test calculation for  $CH_4$  radiative forcing in a mid-latitude summer, clear sky approximation, was made by Grossman et al. (1993) and the result agreed with the Ramanathan et al. (1987) value to within about 4 percent. A calculation of the tropospheric radiative forcing for  $CH_4$  in a globally and annually averaged atmosphere both with and without a representative cloud distribution was made by Grossman and Grant (1993). The results with clouds agreed to within 1 percent of the IPCC (1990) value. These tests indicate that our correlated k-distribution model has the ability to provide consistent tropospheric radiative forcing results. Table 3 shows the radiative forcing values in  $W/m^2$  at representative times between 1 and 30 years after the  $CH_4$  impulse for both the direct  $CH_4$  and the indirect  $O_3$  radiative forcing. Also shown are the results of direct  $CO_2$  tropospheric radiative calculations for year 2 (maximum  $O_3$  radiative forcing) using  $CO_2$  concentrations of 1.29 and 2 times normal  $CO_2$  abundance. The  $CO_2$  calculations were made to test the systematic differences between the IPCC (1990) formula for  $CO_2$  tropospheric radiative forcing and the results obtained using the LLNL model atmosphere. For both cases shown in Table 3 the results of our calculation produce a radiative forcing which is approximately 25 percent higher than that calculated using the IPCC (1990) formula. IPCC (1990) notes that calculations which do not use a cloud cover model, which is the case for our calculations, will result in radiative forcing values which are of the order of 20 percent too high. Thus the agreement of our  $CO_2$  radiative forcing values with the IPCC (1990) values would be of the order of 5 percent if we had included a cloud cover model in our calculations. It is important for the GWP calculations, which will be discussed later, that the  $CO_2$  forcing values derived from the IPCC (1990) formula contain a 25 percent adjustment in order to be comparable with the

$O_3$  and  $CH_4$  forcing values given in Table 3. The results for the time variation of the indirect  $O_3$  radiative forcing, given in Table 3 show that the peak forcing occurs at a time of 2 years after the initial methane impulse. This is indicative of the radiative forcing being correlated with the time variation of the tropospheric ozone column density which peaks at a time of two years (Fig. 5) rather than the total ozone column density which peaks at a time of about 6 years (Fig. 4). The reason for this behavior of the  $O_3$  radiative forcing is that the upward IR flux change is much larger than the downward flux difference at the tropopause at all times and this drives the temporal behavior of the  $O_3$  forcing even though the change in the stratospheric ozone column is much larger than the change in the tropospheric ozone column.

Two interesting aspects of the use of a 2-D latitudinally averaged model atmosphere are the question of the variation of the tropospheric radiative forcing as a function of latitude and the difference between the latitudinally averaged value of the tropospheric radiative forcing and the tropospheric radiative forcing calculated for the globally averaged model atmosphere. We have calculated the direct  $CH_4$  and indirect  $O_3$  tropospheric for five different latitudes between +71 deg. and -71 deg for the time at which maximum  $O_3$  radiative forcing occurs, year 2 after the  $CH_4$  impulse. The results are shown in Table 4. The radiative forcing for  $O_3$  and  $CH_4$  has been shown, for a  $CH_4$  impulse of 2.83 times the concentration of the lowest atmospheric level for each latitude (25 percent of the total tropospheric  $CH_4$  mass), at the actual tropopause at that latitude. There are significant differences between the radiative forcing values calculated in the polar regions and those calculated for the mid latitude and the equatorial regions. The polar values are lower and the mid latitude values are higher than the average value of the forcing. The maximum latitudinal variations are +12, -9 percent for the  $CH_4$  forcing and +29, -49 percent for the  $O_3$  forcing. These excursions from the average may have significant climatalogical consequences which will be discussed later from the point of view of the GWP results. It is interesting to note that the results shown in Table 4 indicate that the radiative forcing values calculated for the globally averaged atmosphere, 0.2455 for  $CH_4$  and 0.1180 for  $O_3$ , differ by ~5 percent ( $CH_4$ ) and ~9 percent ( $O_3$ ) with the average of the forcing values for each latitude. We consider these differences to be small and thus the use of the globally averaged atmosphere to determine the average radiative forcing is a reasonable approach to the GWP calculation.

Table 5 shows the latitude effect of the tropospheric  $CO_2$  radiative forcing for a  $CO_2$  impulse of twice the normal concentration (350 ppm). The  $CO_2$  factor in Table 5 is the ratio of the IPCC (1990) value of the  $CO_2$  forcing ( $4.3668 \text{ W/m}^2$ ) to the  $CO_2$  forcing obtained in this paper (Column 2, Table 5). This factor must be applied to the  $CH_4$  and  $O_3$  forcing results to make them compatible with the IPCC (1990)  $CO_2$  formulation for the GWP calculations to be discussed later. In addition to this factor, the results shown in Table 4 indicate a latitude variation of the direct  $CH_4$  and indirect  $O_3$  radiative forcing. The  $CH_4$  and  $O_3$  factors shown in Table 5 are the product of 1, the ratio of the value of the  $CH_4$  and  $O_3$  tropospheric radiative forcings at the various latitudes to the global average values (Table 4), and 2, the  $CO_2$  factor of Table 5. The variation of these factors represent a rough estimate of the latitude variation of the radiative forcing part of the GWP calculation. The results indicate roughly a  $\pm 10$  percent variation of the  $CH_4$  GWP

with latitude and a larger effect for the O<sub>3</sub> forcing of about 50 percent at the high latitudes.

Table 6 shows the latitude variation of the H<sub>2</sub>O radiative forcing due to changes in the stratospheric H<sub>2</sub>O as well as the latitude averaged value of the radiative forcing. Since H<sub>2</sub>O is a very strong greenhouse gas, the tropopause must be carefully defined since the H<sub>2</sub>O tropospheric radiative forcing will strongly depend on the height of the tropopause. The lower the tropopause the smaller the radiative forcing. In order to compare the latitude averaged radiative forcing for H<sub>2</sub>O with the radiative forcing in a globally averaged atmosphere a test calculation of the radiative forcing in the global averaged atmosphere at year 10 was made. The tropospheric radiative forcing for H<sub>2</sub>O in the globally averaged atmosphere (166 mb tropopause) was approximately 30 percent less than the globally averaged radiative forcing for year 10 given in Table 6. Since the location of the tropopause is a critical factor in the radiative forcing it is recommended, for the case of H<sub>2</sub>O forcing, that the radiative forcing should be calculated as a function of latitude and then averaged as opposed to the calculation of the radiative forcing in the globally averaged atmosphere.

### B. UV Effects On O<sub>3</sub> Radiative Forcing

Since O<sub>3</sub> has an absorption band in the UV spectral region the possibility exists that there may be a significant contribution to the total radiative forcing by the differential UV absorption. We make an estimation of the UV radiation forcing contribution in the following manner. The atmosphere is considered as a two component system. The stratosphere is taken to be a pure absorption region while the troposphere is taken to be a scattering and absorbing layer. The spectral region over which the UV radiative forcing will be calculated is taken to be 250–340 nm in 5 nm spectral sub intervals. The O<sub>3</sub> absorption cross sections and Rayleigh scattering cross sections are given by WMO-16 (1985). The radiative forcing calculation is done for the year 2 model atmosphere (the maximum O<sub>3</sub> forcing model). The downward UV flux at the tropopause is calculated using a simple Beer's Law exponential attenuation of the zero air mass solar flux (Goody and Yung, 1989). The upward flux at the tropopause is calculated using a delta-Eddington scattering model in the troposphere which takes the troposphere as a single scattering layer. In addition to the diffuse, reflected flux component from the troposphere additional upward flux components due to the attenuated direct and downward scattered beams that are reflected from the ground are also considered. The ground albedo was taken to be 0.2. The UV radiative forcing calculated in this way amounted to about 9 percent of the IR radiative forcing. Thus UV forcing effects should be a 10 percent effect at most.

## IV. Carbon Cycle Model and CO<sub>2</sub> Response Curves.

Unlike many of the greenhouse gases emitted to the atmosphere, CO<sub>2</sub> does not have a chemical or photochemical sink within the troposphere or stratosphere. Removal of CO<sub>2</sub> is therefore dependent on exchanges with other carbon reservoirs. Following the emissions of a hypothetical pulse of CO<sub>2</sub> into the atmosphere, about 10% will be removed within 2 to 3 years through gaseous diffusion into the mixed layer of the ocean.

Subsequent removal is dependent on downward mixing into the deeper ocean. Ultimately, the rest of the initial pulse can be removed by mixing into the ocean, but only over a time period of hundreds of years (Maier-Reimer and Hasselmann, 1987). To avoid the need to use a single lifetime for CO<sub>2</sub>, we have used a coupled climate-carbon cycle model of Jain and Bach (1994) to calculate the decay rate of CO<sub>2</sub>. This model contains a box-diffusion carbon cycle model consisting of three reservoirs, namely the atmosphere, the mixed ocean layer (ca. 75 m) and the deep ocean (ca. 4000 m). The model ocean is treated as a diffusive medium with constant vertical eddy diffusivity. The model also takes into account the interaction with the biosphere. The biospheric emissions are calculated by a multi-box globally aggregated terrestrial biosphere submodel developed by Harvey (1989). The model includes stimulation of net photosynthesis or net primary productivity by enhanced atmospheric CO<sub>2</sub> using the fertilization factor  $\beta$ .

To correctly estimate the GWP values and the past and future CO<sub>2</sub> concentrations, it is important to use carbon cycle models that properly balance the carbon budget. To balance the carbon cycle means to remove any inconsistencies between model output and observations. When a balanced model is run from pre-industrial times to the current date using the observed emissions, it will give the correct history of CO<sub>2</sub> concentration changes. However, the carbon cycle model used to calculate the GWPs given by IPCC (1990, 1992) does not properly balance the carbon budget. In a separate study (Wuebbles et al., 1993) we have assessed the effects of balancing the carbon budget on GWP values. The CO<sub>2</sub> variations can be made to fit observations by assuming the larger ocean flux, and/or accounting for feedbacks in the terrestrial component of the carbon cycle and/or assuming the existence of an additional CO<sub>2</sub> sink. The present model is sufficiently flexible that all three methods may be used; we chose to use only the first two methods. In Figure 7, the observed CO<sub>2</sub> concentrations are compared with the results of the carbon cycle model. The carbon cycle model including the biospheric feedbacks satisfactorily reproduces the observed atmospheric CO<sub>2</sub> concentration (balanced case). Excluding the effects of the biosphere (i.e. unbalanced case) results in an overestimation of CO<sub>2</sub> concentration. The time variation of the fraction of CO<sub>2</sub> concentration remaining after an atmospheric impulse is shown in Figure 8. It will be used in the GWP calculation described in the following section.

## V. Global Warming Potential Model

### A. Basic Model

Global warming potentials (GWPs) are evaluated according to the concept of IPCC (1990). A concentration change of trace gas X, arising from an impulse of a unit mass of the trace gas X (for direct GWPs) or from chemical processing due to an impulse of gas Y (for indirect GWPs), in the atmosphere produces a tropospheric radiative forcing change  $\Delta f_X(t)$ , which decreases with time as X is removed from the atmosphere. This radiative forcing change is considered as directly proportional to the temperature change at the surface via a climate sensitivity factor. Commitment to radiative forcing from a unit mass of X is the integral of  $\Delta f_X(t)$  from the time of an impulse to the user-selected GWP time horizon, T. The GWP of X is the radiative forcing commitment from a unit mass of

X divided by the radiative forcing commitment from a unit mass of CO<sub>2</sub>, or a CO<sub>2</sub> like molecule,

$$GWP_X = \frac{\int_0^T \Delta f_X(t) dt}{\int_0^T \Delta f_{CO_2}(t) dt} \quad (2)$$

The IPCC (1990)-derived GWPs assume that the background atmosphere is in equilibrium (that background concentrations are constant over the GWP integration period). In our calculations, the chemical processes are allowed to operate on the background concentrations for the trace gases that are present in the atmosphere just before the impulse. This has, as will be discussed later, a significant effect on the equivalent lifetime of the decay of the impulse of the trace gas X to the atmosphere.

The definition of GWP (1990) requires integration of radiative forcing (or tropospheric temperature change) resulting from a unit mass release of trace gas, usually one kilogram, and of CO<sub>2</sub>. A small change in atmospheric concentration resulting from such a small release can produce computational errors, so larger mass releases are usually applied and then the radiative forcing is scaled to a one kilogram release. Radiative forcing scales linearly for many gases at reasonable concentrations (IPCC, 1990); only for releases of gas much greater than one gigaton of CO<sub>2</sub>, CH<sub>4</sub>, or N<sub>2</sub>O does nonlinearity occur (Wuebbles *et al.*, 1993). The radiative forcing of CO<sub>2</sub> is obtained from the IPCC (1990) formula,

$$\Delta F_{CO_2} = 6.3 \log_e \left( \frac{c_{CO_2}(t)}{c_{CO_2}^0} \right) \quad (3)$$

for which  $c_{CO_2}(t)$  is the concentration of CO<sub>2</sub> at time t and  $c_{CO_2}^0$  is the concentration of CO<sub>2</sub> which would exist in the absence of the pulse. In the equilibrium case used here,  $c_{CO_2}^0$  is constant with respect to time, so that the argument of the log<sub>e</sub> is replaced by one plus the impulse response function for CO<sub>2</sub>,  $i_{CO_2}(t)$ :

$$\begin{aligned} \Delta F_{CO_2} &= 6.3 \log_e (1 + i_{CO_2}(t)); \\ i_{CO_2}(t) &= \frac{c_{CO_2}(t) - c_{CO_2}^0}{c_{CO_2}^0} \end{aligned} \quad (4)$$

The impulse response function used in this study was discussed in the previous section (Figure 8). Mass-scaled, integrated radiative forcing for CO<sub>2</sub> is then calculated by the procedure described in Wuebbles *et al.* (1993) at time horizons of 20, 50, 100, 200, and 500 yr.

## B. Extrapolation and integration of radiative forcing

The radiative forcing values of Tables 3 and 6 must be fitted before numerical integration in Equation 2 due to the uneven timestep required by computer limitations and to time horizons exceeding the longest time after pulse for which the atmospheric and line models were run. IPCC (1990) states that CH<sub>4</sub> radiative forcings are proportional to  $c_{CH_4}(t)^{1/2}$ , while tropospheric O<sub>3</sub> radiative forcings are linear in  $c_{O_3}(t)$ . In turn, the concentration perturbations of the two trace species may be taken as negative exponentials in time t. However, as seen by Figures 9 and 10, the initially perturbed atmosphere produces concentrations inconsistent with a negative exponential in t. Points for which this is the case, the first year of the CH<sub>4</sub> radiative forcings and years 1–4 after the pulse for O<sub>3</sub>, are excluded from fitting for this reason. The fits after weighting by CH<sub>4</sub> mass are:

$$\Delta f_{CH_4} = (\exp(-58.841 \pm 0.028 - 0.1189 \pm 0.0024 t))^{1/2}, \quad (5a)$$

$$\Delta f_{O_3} = \exp(-30.0410 \pm 0.0035 - 0.05663 \pm 0.00022 t), \quad (5b)$$

$$\Delta f_{H_2O} = \exp(-3.9645 \pm 0.040 - (0.05991 \pm 0.0017)t). \quad (5c)$$

For the integration of the radiative forcing of CH<sub>4</sub>, the value in Table 3 is used for the first year after the pulse. Years 1 to 3 after the pulse also are used in the O<sub>3</sub> Δf integration, and the value at year 4 is replaced by a linear interpolation of years 3 and 5. Fit values are used for all years afterward. Simpson's Rule (Press et al., 1992, equ. 4.1.13) is then applied to integrate the radiative forcing over time. The radiative forcing for zero time after the pulse is set to zero in each case for integration. Integrated radiative forcings for CH<sub>4</sub>, H<sub>2</sub>O, and O<sub>3</sub> are each multiplied by a factor of 0.8 to reconcile the clear sky approximation with the IPCC (1990) cloud parameterization as discussed previously. Table 7 lists the integrated radiative forcings per kilogram derived for each of the gases.

## C. GWP Results

Table 8 shows the results of the GWP calculations. The CH<sub>4</sub> GWP values are significantly larger than those given by IPCC (1990, 1992) and Wuebbles et al. (1993). In the IPCC calculations the CH<sub>4</sub> lifetime was given as 10.5 years, which implies that the OH abundance was held fixed at the ambient value. In the present calculation, the chemical processes which affect CH<sub>4</sub>, O<sub>3</sub>, and H<sub>2</sub>O abundances are allowed operate and as a result the OH abundance changes as the chemical equilibrium is perturbed by the CH<sub>4</sub> pulse. Equation 1 predicts a lifetime of CH<sub>4</sub> which is dependent on the OH abundance. This long apparent lifetime of the pulse is the result of the slower destruction of all CH<sub>4</sub> from the decrease in OH. The radiative forcing fits for CH<sub>4</sub> given by Equation 5a and shown in Figure 9 indicate an apparent lifetime on the order of 17 years for the decay of the CH<sub>4</sub> pulse. Wuebbles et al. (1992) showed that when the CH<sub>4</sub> lifetime is increased, the GWP values also increase towards the results obtained in the present

calculation. For a lifetime of 12.6 years, GWP's at 20, 100, and 500 years of 41.7, 15.9, and 7.1 were obtained. A simple extrapolation of the GWP vs. CH<sub>4</sub> lifetime results Wuebbles et al. (1992) predicts a GWP of approximately 52 at 20 years which is the same as that obtained in this paper. The results obtained for the O<sub>3</sub> indirect radiative forcing are on the order of 10 to 20 percent higher than those given in IPCC (1990) and Wuebbles et al. (1993). Given the uncertainties of the calculations, at least 20 to 30 percent, this is a reasonable agreement. The indirect GWP's for stratospheric H<sub>2</sub>O obtained in this paper are lower by factors of 3 to 5 than those given in IPCC (1990). This is probably due to an overestimation of the tropospheric radiative forcing of H<sub>2</sub>O in IPCC (1990). The ratio of the indirect H<sub>2</sub>O GWP to the direct CH<sub>4</sub> GWP, for the calculations in this paper is about 4 percent and agrees quite well with the results obtained by Lelieveld and Crutzen (1992) who give a value of 5 percent for this ratio. This effect is strongly dependent on the height of the tropopause since H<sub>2</sub>O is such a strong IR absorber and should have a sharp mixing ratio gradient at the tropopause. The overall uncertainty in the GWP calculations is due to the uncertainties in the lifetime of CH<sub>4</sub>, the amount of NO<sub>x</sub> present in the atmosphere, and the radiative forcing calculations. The best estimate of the overall uncertainty in the calculations is on the order of 20 percent.

## **VI. Conclusions**

We have calculated the direct CH<sub>4</sub> GWP and the indirect O<sub>3</sub> and stratospheric H<sub>2</sub>O GWPs resulting from a CH<sub>4</sub> pulse equal to ~36 percent of the total atmospheric mass of CH<sub>4</sub>. The direct CH<sub>4</sub> GWP is significantly larger than previous estimates as a result of the effect on the pulse response time due to the variation of the OH abundance. The agreement of the indirect O<sub>3</sub> GWP effect with previous estimates is within the uncertainty bounds of the calculation. The indirect H<sub>2</sub>O GWP is much less than the estimate given in IPCC (1990, 1992) but agrees very well with more recent calculations Lelieveld and Crutzen (1992). The H<sub>2</sub>O effect is very strongly dependent on the location of the tropopause because of the strong IR absorption of H<sub>2</sub>O. Future calculations need to be made to determine the effect of the magnitude of the CH<sub>4</sub> impulse on the impulse decay time and the effect of the presence of hydrocarbons and NO<sub>x</sub> on the direct and indirect GWP's.

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## **Figure Captions**

Figure 1. Globally and annually averaged profiles of water vapor, ozone, and methane as a function of altitude for the ambient atmosphere.

Figure 2. Pressure-temperature profile for the ambient atmosphere. The temperatures are globally and annually averaged.

Figure 3. Total mass of methane (in units of teragrams) in the model atmosphere as a function of time before and after a pulse emission of methane equal to the equilibrium increase of CH<sub>4</sub> produced by a constant 25% increase in total emissions. Feedbacks in the lifetime of methane result in about a 36% peak increase in total atmospheric methane. The ambient value of the methane mass is indicated by the dashed line.

Figure 4. Annual average total ozone column after the pulse increase of methane. The ambient value of the ozone column is indicated by the dashed line.

Figure 5. Annually averaged tropospheric ozone column after the pulse increase of methane. The ambient value of the troposperic ozone column is indicated by the dashed line.

Figure 6. Increase in annually averaged stratospheric water vapor burden (kg) before and after the pulse emission of methane.

Figure 7. The time variation of the observed CO<sub>2</sub> concentration (+), the carbon cycle model prediction including biospheric feedbacks (—), and the carbon cycle model prediction excluding the biosphere (----).

Figure 8. The response of atmospheric CO<sub>2</sub> to a pulse of 1 GTC (gigatons of Carbon).

Figure 9. Radiative forcing of methane vs. time (years) after the pulse emission of methane. The correlated k-distribution radiative forcing model calculations are denoted by the symbols. The solid line is the fit to the model calculations given by Equation 4.

Figure 10. Radiative forcing of ozone vs. time (years) after the pulse emission of methane. The correlated k-distribution radiative forcing model calculations are denoted by the symbols. The solid line is the fit to the model calculations given by Equation 4.

**Table 1.** Chemical reaction mechanism for LLNL two-dimensional model. The reference used for all photochemical data is Demore et al. (1992).

(a) Two-body reactions (Arrhenius rate constant expression  $k = A \cdot \exp\left(\frac{-E}{RT}\right)$ )

No.	Reaction	A <sup>1</sup>	E/R <sup>2</sup>
1	O + O <sub>3</sub> → 2*O <sub>2</sub>	8.00E-12	2,060
2	O <sub>1</sub> D + N <sub>2</sub> → O + N <sub>2</sub>	1.80E-11	-110
3	O <sub>1</sub> D + O <sub>2</sub> → O + O <sub>2</sub>	3.20E-11	-70
4	O <sub>1</sub> D + O <sub>3</sub> → 2*O <sub>2</sub>	1.20E-10	0
5	O <sub>1</sub> D + O <sub>3</sub> → O <sub>2</sub> + 2*O	1.20E-10	0
6	H <sub>2</sub> O + O <sub>1</sub> D → 2*OH	2.20E-10	0
7	H <sub>2</sub> + O <sub>1</sub> D → OH + H	1.00E-10	0
8	N <sub>2</sub> O + O <sub>1</sub> D → N <sub>2</sub> + O <sub>2</sub>	4.90E-11	0
9	N <sub>2</sub> O + O <sub>1</sub> D → 2*NO	6.70E-11	0
10	CH <sub>4</sub> + O <sub>1</sub> D → CH <sub>2</sub> O + H <sub>2</sub>	1.40E-11	0
11	CH <sub>4</sub> + O <sub>1</sub> D → CH <sub>3</sub> O <sub>2</sub> + OH	1.40E-10	0
12	CF <sub>2</sub> Cl <sub>2</sub> + O <sub>1</sub> D → 2*Cl	1.12E-10	0
13	CF <sub>3</sub> CCl <sub>3</sub> + O <sub>1</sub> D → 3*Cl	1.60E-10	0
14	CF <sub>3</sub> CFCl <sub>2</sub> + O <sub>1</sub> D → 2*Cl	1.28E-10	0
15	CF <sub>3</sub> CF <sub>2</sub> Cl + O <sub>1</sub> D → Cl	7.12E-11	0
16	CHF <sub>2</sub> Cl + O <sub>1</sub> D → Cl	7.00E-11	0
17	H + O <sub>3</sub> → OH + O <sub>2</sub>	1.40E-10	470
18	H <sub>2</sub> + OH → H <sub>2</sub> O + H	5.50E-12	2,000
19	OH + O <sub>3</sub> → HO <sub>2</sub> + O <sub>2</sub>	1.60E-12	940
20	OH + O → O <sub>2</sub> + H	2.20E-11	-120
21	HO <sub>2</sub> + O → OH + O <sub>2</sub>	3.00E-11	-200
22	HO <sub>2</sub> + O <sub>3</sub> → OH + 2*O <sub>2</sub>	1.10E-14	500
23	HO <sub>2</sub> + OH → H <sub>2</sub> O + O <sub>2</sub>	4.80E-11	-250
24	H <sub>2</sub> O <sub>2</sub> + OH → H <sub>2</sub> O + HO <sub>2</sub>	2.90E-12	160
25	N + O <sub>2</sub> → NO + O	1.50E-11	3,600
26	N + NO → N <sub>2</sub> + O	3.40E-11	0
27	NO + O <sub>3</sub> → NO <sub>2</sub> + O <sub>2</sub>	2.00E-12	1,400
28	NO + HO <sub>2</sub> → NO <sub>2</sub> + OH	3.70E-12	-250
29	NO <sub>2</sub> + O → NO + O <sub>2</sub>	6.50E-12	-120
30	NO <sub>2</sub> + O <sub>3</sub> → NO <sub>3</sub> + O <sub>2</sub>	1.20E-13	2,450
31	N <sub>2</sub> O <sub>5</sub> + H <sub>2</sub> O → 2*HNO <sub>3</sub>	5.00E-22	0
32	HO <sub>2</sub> NO <sub>2</sub> + OH → H <sub>2</sub> O + NO <sub>2</sub> + O <sub>2</sub>	1.30E-12	-380
33	Cl + O <sub>3</sub> → ClO + O <sub>2</sub>	2.90E-11	260
34	Cl + HO <sub>2</sub> → HCl + O <sub>2</sub>	1.80E-11	-170
35	Cl + HO <sub>2</sub> → OH + ClO	4.10E-11	450
36	ClO + O → Cl + O <sub>2</sub>	3.00E-11	-70
37	ClO + OH → HO <sub>2</sub> + Cl	1.10E-11	-120
38	ClO + HO <sub>2</sub> → O <sub>2</sub> + HOCl	4.80E-13	-700
39	ClO + NO → NO <sub>2</sub> + Cl	6.40E-12	-290
40	ClO + ClO → Cl + ClOO	4.00E-13	1,250
41	ClO + ClO → Cl <sub>2</sub> + O <sub>2</sub>	4.00E-13	1,250

<sup>1</sup> Units are cm<sup>3</sup>/molecule-sec.

<sup>2</sup> Unit is degrees Kelvin.

No.	Reaction	A <sup>3</sup>	E/R <sup>4</sup>
42	OCIO + Cl → 2*ClO	3.40E-11	-160
43	OCIO + O → O <sub>2</sub> + ClO	2.50E-12	950
44	OCIO + OH → HOCl + O <sub>2</sub>	4.50E-13	-800
45	OCIO + NO → NO <sub>2</sub> + ClO	2.50E-12	600
46	ClOO + Cl → Cl <sub>2</sub> + O <sub>2</sub>	2.30E-10	0
47	Cl <sub>2</sub> O <sub>2</sub> + Cl → Cl <sub>2</sub> + ClOO	1.00E-10	0
48	HCl + OH → H <sub>2</sub> O + Cl	2.60E-12	350
49	HOCl + OH → H <sub>2</sub> O + ClO	3.00E-12	500
50	ClONO <sub>2</sub> + O → ClO + NO + O <sub>2</sub>	3.19E-13	800
51	ClONO <sub>2</sub> + O → ClO + NO <sub>2</sub> + O	2.58E-12	800
52	ClONO <sub>2</sub> + OH → HOCl + NO + O <sub>2</sub>	1.32E-13	333
53	ClONO <sub>2</sub> + OH → HOCl + NO <sub>2</sub> + O	1.07E-12	333
54	ClONO <sub>2</sub> + Cl → Cl <sub>2</sub> + NO + O <sub>2</sub>	7.48E-13	-160
55	ClONO <sub>2</sub> + Cl → Cl <sub>2</sub> + NO <sub>2</sub> + O	6.05E-12	-160
56	Br + O <sub>3</sub> → BrO + O <sub>2</sub>	1.70E-11	800
57	Br + HO <sub>2</sub> → HBr + O <sub>2</sub>	1.50E-11	600
58	Br + NO <sub>3</sub> → BrO + NO <sub>2</sub>	1.60E-11	0
59	Br + OCIO → BrO + ClO	2.60E-11	1,300
60	Br + Cl <sub>2</sub> O <sub>2</sub> → BrCl + ClOO	3.00E-12	0
61	Br + CH <sub>2</sub> O → HBr + HO <sub>2</sub> + CO	1.70E-11	800
62	BrO + O → Br + O <sub>2</sub>	3.00E-11	0
63	BrO + HO <sub>2</sub> → HOBr + O <sub>2</sub>	6.20E-12	-500
64	BrO + OH → Br + HO <sub>2</sub>	1.10E-11	0
65	BrO + NO → Br + NO <sub>2</sub>	8.80E-12	-260
66	BrO + NO <sub>3</sub> → NO <sub>2</sub> + Br + O <sub>2</sub>	1.00E-12	0
67	BrO + ClO → Br + OCIO	1.60E-12	-430
68	BrO + ClO → Br + ClOO	2.90E-12	-220
69	BrO + ClO → BrCl + O <sub>2</sub>	5.80E-13	-170
70	BrO + BrO → 2*Br + O <sub>2</sub>	1.40E-12	-150
71	HBr + O → Br + OH	5.80E-12	1,500
72	HBr + OH → Br + H <sub>2</sub> O	1.10E-11	0
73	CH <sub>4</sub> + OH → CH <sub>3</sub> O <sub>2</sub> + H <sub>2</sub> O	2.90E-12	1,820
74	CH <sub>2</sub> O + OH → H <sub>2</sub> O + HO <sub>2</sub> + CO	1.00E-11	0
75	CH <sub>3</sub> O <sub>2</sub> + O → CH <sub>2</sub> O + HO <sub>2</sub>	3.00E-11	0
76	CH <sub>2</sub> O + O → HO <sub>2</sub> + OH + CO	3.40E-11	1,600
77	CH <sub>3</sub> O <sub>2</sub> + NO → HO <sub>2</sub> + CH <sub>2</sub> O + NO <sub>2</sub>	4.20E-12	-180
78	Cl + CH <sub>4</sub> → CH <sub>3</sub> O <sub>2</sub> + HCl	1.10E-11	1,400
79	Cl + CH <sub>2</sub> O → HCl + HO <sub>2</sub> + CO	8.10E-11	30
80	CH <sub>3</sub> Cl + OH → Cl + H <sub>2</sub> O + HO <sub>2</sub>	2.10E-12	1,150
81	CH <sub>3</sub> CCl <sub>3</sub> + OH → H <sub>2</sub> O + 3*Cl	1.80E-12	1,550
82	CHF <sub>2</sub> Cl + OH → Cl + H <sub>2</sub> O	1.20E-12	1,650
83	CH <sub>3</sub> Cl + Cl → HO <sub>2</sub> + CO + 2*HCl	3.30E-11	1,250
84	CH <sub>3</sub> Br + OH → Br + H <sub>2</sub> O	3.60E-12	1,430

<sup>3</sup>Units are cm<sup>3</sup>/molecule-sec.

<sup>4</sup>Unit is degrees Kelvin.

(b) Three-body reactions (special rate constant expressions such as Troë equation)

Number	Reaction
1	$O + O_2 \rightarrow O_3$
2	$H + O_2 \rightarrow HO_2$
3	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$
4	$HO_2 + HO_2 + H_2O \rightarrow H_2O_2 + O_2 + H_2O$
5	$NO_2 + HO_2 \rightarrow HO_2NO_2$
6	$NO_3 + NO_2 \rightarrow N_2O_5$
7	$N_2O_5 \rightarrow NO_2 + NO_3$
8	$NO_2 + OH \rightarrow HNO_3$
9	$HNO_3 + OH \rightarrow H_2O + NO + O_2$
10	$HNO_3 + OH \rightarrow H_2O + NO_2 + O$
11	$HO_2NO_2 \rightarrow HO_2 + NO_2$
12	$ClO + NO_2 \rightarrow ClONO_2$
13	$ClO + ClO \rightarrow Cl_2O_2$
14	$ClOO \rightarrow Cl + O_2$
15	$Cl_2O_2 \rightarrow 2^*ClO$
16	$BrO + NO_2 \rightarrow BrONO_2$
17	$CO + OH \rightarrow H$
18	$N_2O_5 \rightarrow 2^*HNO_3$
19	$ClONO_2 \rightarrow HOCl + HNO_3$

(c) Photolysis reactions

Number	Reaction
1.	$O_2 + h\nu \rightarrow 2^*O$
2.	$O_3 + h\nu \rightarrow O + O_2$
3.	$O_3 + h\nu \rightarrow O_1D + O_2$
4.	$H_2O_2 + h\nu \rightarrow 2^*OH$
5.	$H_2O + h\nu \rightarrow H + OH$
6.	$NO_2 + h\nu \rightarrow NO + O$
7.	$N_2O + h\nu \rightarrow N_2 + O_1D$
8.	$NO + h\nu \rightarrow N + O$
9.	$NO_3 + h\nu \rightarrow NO_2 + O$
10.	$NO_3 + h\nu \rightarrow NO + O_2$
11.	$N_2O_5 + h\nu \rightarrow NO_2 + NO + O_2$
12.	$N_2O_5 + h\nu \rightarrow 2^*NO_2 + O$
13.	$N_2O_5 + h\nu \rightarrow NO_2 + NO + 2^*O$
14.	$N_2O_5 + h\nu \rightarrow 2^*NO + O_2 + O$
15.	$HNO_3 + h\nu \rightarrow OH + NO_2$
16.	$HO_2NO_2 + h\nu \rightarrow OH + NO + O_2$
17.	$HO_2NO_2 + h\nu \rightarrow OH + NO_2 + O$
18.	$HO_2NO_2 + h\nu \rightarrow HO_2 + NO_2$
19.	$Cl_2 + h\nu \rightarrow 2^*Cl$
20.	$ClO + h\nu \rightarrow Cl + O$
21.	$ClO + h\nu \rightarrow Cl + O_1D$
22.	$OCIO + h\nu \rightarrow O + ClO$
23.	$ClOO + h\nu \rightarrow ClO + O$
24.	$Cl_2O_2 + h\nu \rightarrow Cl + ClOO$
25.	$HOCl + h\nu \rightarrow OH + Cl$
26.	$ClONO_2 + h\nu \rightarrow Cl + NO + O_2$
27.	$ClONO_2 + h\nu \rightarrow Cl + NO_2 + O$
28.	$ClONO_2 + h\nu \rightarrow Cl + NO_2 + O$
29.	$BrCl + h\nu \rightarrow Br + Cl$
30.	$BrO + h\nu \rightarrow Br + O$
31.	$HBr + h\nu \rightarrow H + Br$
32.	$HOBr + h\nu \rightarrow Br + OH$
33.	$BrONO_2 + h\nu \rightarrow Br + NO_2 + O$
34.	$BrONO_2 + h\nu \rightarrow Br + NO + O_2$
35.	$CH_2O + h\nu \rightarrow CO + H_2$
36.	$CH_2O + h\nu \rightarrow HO_2 + CO + H$
37.	$CH_3Cl + h\nu \rightarrow CH_3O_2 + Cl$
38.	$CCl_4 + h\nu \rightarrow 4^*Cl$
39.	$CH_3CCl_3 + h\nu \rightarrow 3^*Cl$
40.	$CFCI_3 + h\nu \rightarrow 3^*Cl$
41.	$CF_2Cl_2 + h\nu \rightarrow 2^*Cl$
42.	$CF_3CCl_3 + h\nu \rightarrow 3^*Cl$
43.	$CF_3CFCI_2 + h\nu \rightarrow 2^*Cl$
44.	$CF_3CF_2Cl + h\nu \rightarrow Cl$
45.	$CHF_2Cl + h\nu \rightarrow Cl$
46.	$CH_3Br + h\nu \rightarrow Br + CH_3O_2$
47.	$CF_3Br + h\nu \rightarrow Br$
48.	$CF_2ClBr + h\nu \rightarrow Br + Cl$

**Table 2.** Surface emission inventory for the LLNL two-dimensional model. (teragrams per year)

Model Zone	Latitude Center	Methane	Carbon Monoxide	Nitrogen Dioxide
1	-80.1	0.00	0.60	0.00
2	-70.9	0.00	1.00	0.00
3	-62.3	0.00	8.45	0.00
4	-53.1	0.15	18.64	1.98
5	-42.5	4.08	35.62	7.27
6	-30.0	18.99	84.83	10.35
7	-17.5	24.67	136.09	15.63
8	-5.7	39.25	154.50	11.67
9	5.7	42.43	145.11	12.67
10	17.5	54.99	167.10	10.69
11	30.0	81.71	197.88	20.37
12	42.5	70.41	209.05	27.09
13	53.1	57.51	126.63	8.88
14	62.3	30.00	34.40	4.83
15	70.9	15.92	5.02	0.00
16	80.1	12.77	3.01	0.00
TOTALS (Tg/yr):		452.9	1328	131.4

**Table 3.** Radiative Forcing W/m<sup>2</sup>

Year	Direct CH <sub>4</sub>	Indirect O <sub>3</sub>	CO <sub>2</sub> (1.29)	CO <sub>2</sub> (2.0)
1	0.2500	0.0947		
2	0.2455	0.1180	1.956	5.453
3	0.2312	0.1165		
6	0.1950	0.1013		
7	0.1844	0.0957		
8	0.1744	0.0909		
9	0.1649	0.0861		
10	0.1558	0.0818		
15	0.1176	0.0614		
20	0.0884	0.0462		
25	0.0665	0.0348		
30	0.0500	0.0261		

**Table 4.** Latitude Variation Of Radiative Forcing (W/M<sup>2</sup>) For Year 2

LATITUDE (DEG)	DIRECT CH <sub>4</sub> (P. TROP.)	INDIRECT O <sub>3</sub> (P. TROP.)
-71	0.2403 (292mb)	0.0625 (292mb)
-30	0.2755 (139mb)	0.1518 (139mb)
+5.7	0.2628 (123mb)	0.1516 (123mb)
+30	0.2659 (135mb)	0.1406 (135mb)
+71	0.2244 (302mb)	0.0603 (302mb)
Avg.	0.2603	0.1297
% Diff.	+5 (0.2455)	+9 (0.1180)

**Table 5.** Latitude Effect Of CO<sub>2</sub> Forcing For An Impulse Doubling Of CO<sub>2</sub>

LATITUDE	FORCING (W/m <sup>2</sup> )	CO <sub>2</sub> FACTOR	CH <sub>4</sub> FACTOR	O <sub>3</sub> FACTOR
Average	5.453	0.8	0.8	0.8
-71	4.418	0.988	0.967	0.523
-30	5.735	0.76	0.852	0.977
+5.7	5.976	0.73	0.781	0.939
+30	5.773	0.76	0.823	0.906
+71	4.624	0.944	0.863	0.482

**Table 6.** Latitude Variation Of H<sub>2</sub>O Radiative Forcing (W/M<sup>2</sup>)

LATITUDE (DEG)	H <sub>2</sub> O Forcing		
	Year 5	Year 10	Year 20
-60 (278mb)	2.085 (-3)	5.302 (-3)	3.761 (-3)
-30 (139mb)	4.179 (-3)	1.021 (-3)	7.270 (-3)
Eq. (123mb)	2.995 (-3)	6.456 (-3)	4.715 (-3)
+30 (135mb)	5.295 (-3)	1.251 (-2)	8.911 (-3)
+60 (278mb)	1.741 (-3)	4.032 (-3)	2.932 (-3)
Avg.	3.629 (-3)	8.535 (-3)	6.099 (-3)

**Table 7.** Radiative Forcing Integrals per Kilogram Mass of the Trace Gases

	20 yr	50 yr	100 yr	200 yr	500 yr
CH <sub>4</sub>	1.505e-12 <sup>a</sup>	2.074e-12	2.183e-12	b	b
O <sub>3</sub> (CH <sub>4</sub> )	7.931e-13	1.127e-12	1.198e-12	b	b
H <sub>2</sub> O(CH <sub>4</sub> )	5.624e-14		1.012e-13		1.016e-13
CO <sub>2</sub>	3.117e-14	6.303e-14	1.073e-13	1.832e-13	3.612e-13

<sup>a</sup>Read "e-" as an exponent, thus  $1.505\text{e-}12 = 1.505 \times 10^{-12}$ . Units are  $\text{W yr m}^2 \text{kg}^{-1}$  at the tropopause.

<sup>b</sup>Taken as identical to the value for time horizon of 100 yr.

**Table 8.** Global Warming Potentials and the Indirect GWP Total Uncertainty Estimate

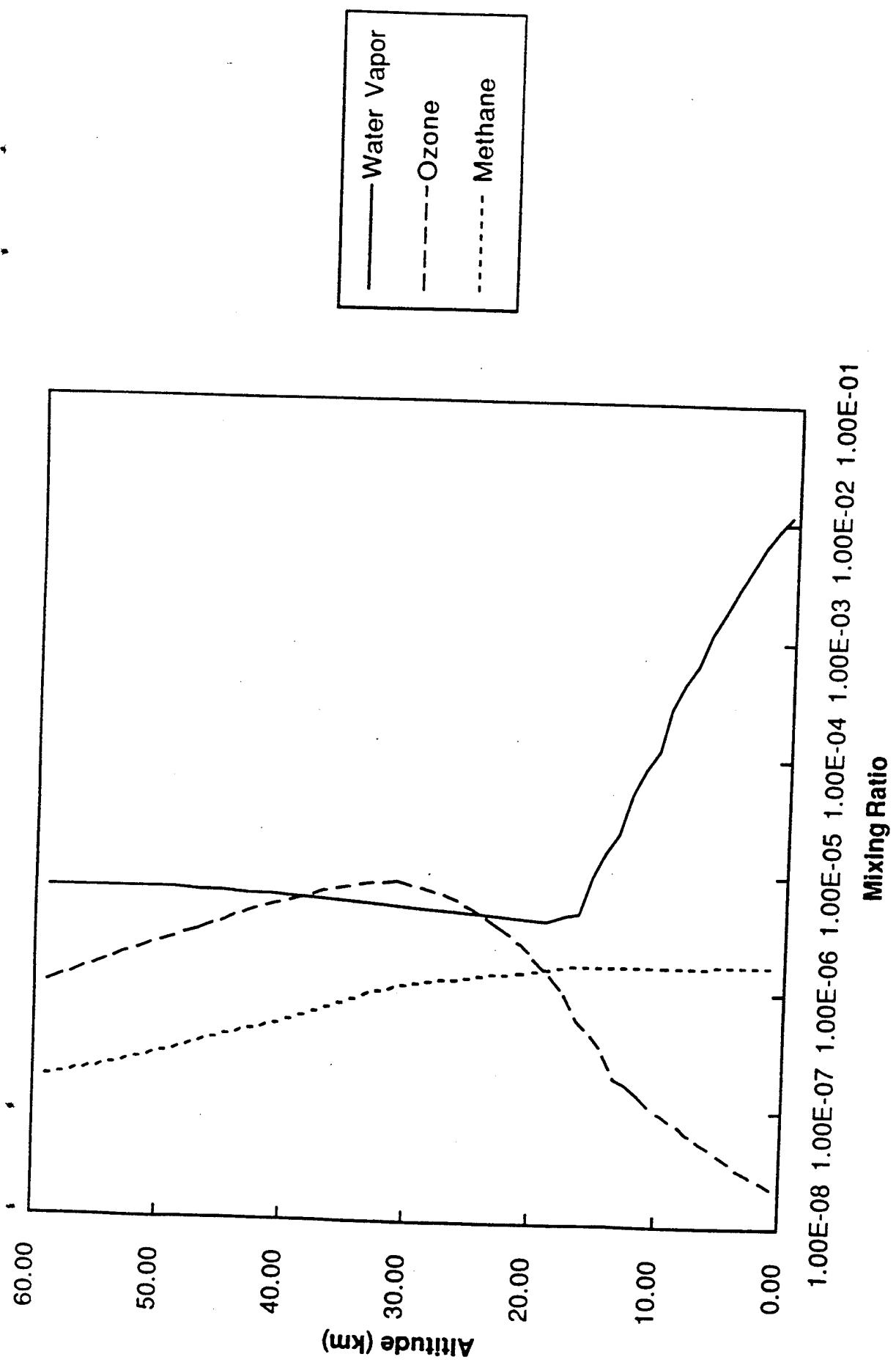
	source	20 yr	50 yr	100 yr	200 yr	500 yr
CH <sub>4</sub>	current	52.6		22.9		7.0
	a	37.7	21.7	12.9	7.5	3.8
	b	34		9		2
	c	35		11		4
O <sub>3</sub> (CH <sub>4</sub> )	current	26.7		11.7		3.58
	b	24		8		3
	a	23.1		10.4		3.1
H <sub>2</sub> O(CH <sub>4</sub> )	current	1.9		1.01		0.31
	b	10		4		1

## Sources:

(a) Wuebbles *et al.*, 1993

(b) IPCC, 1990

(c) IPCC, 1992.



**Figure 1** Globally- and annually-averaged profiles of water vapor, ozone, and methane as a function of altitude for the ambient atmosphere.

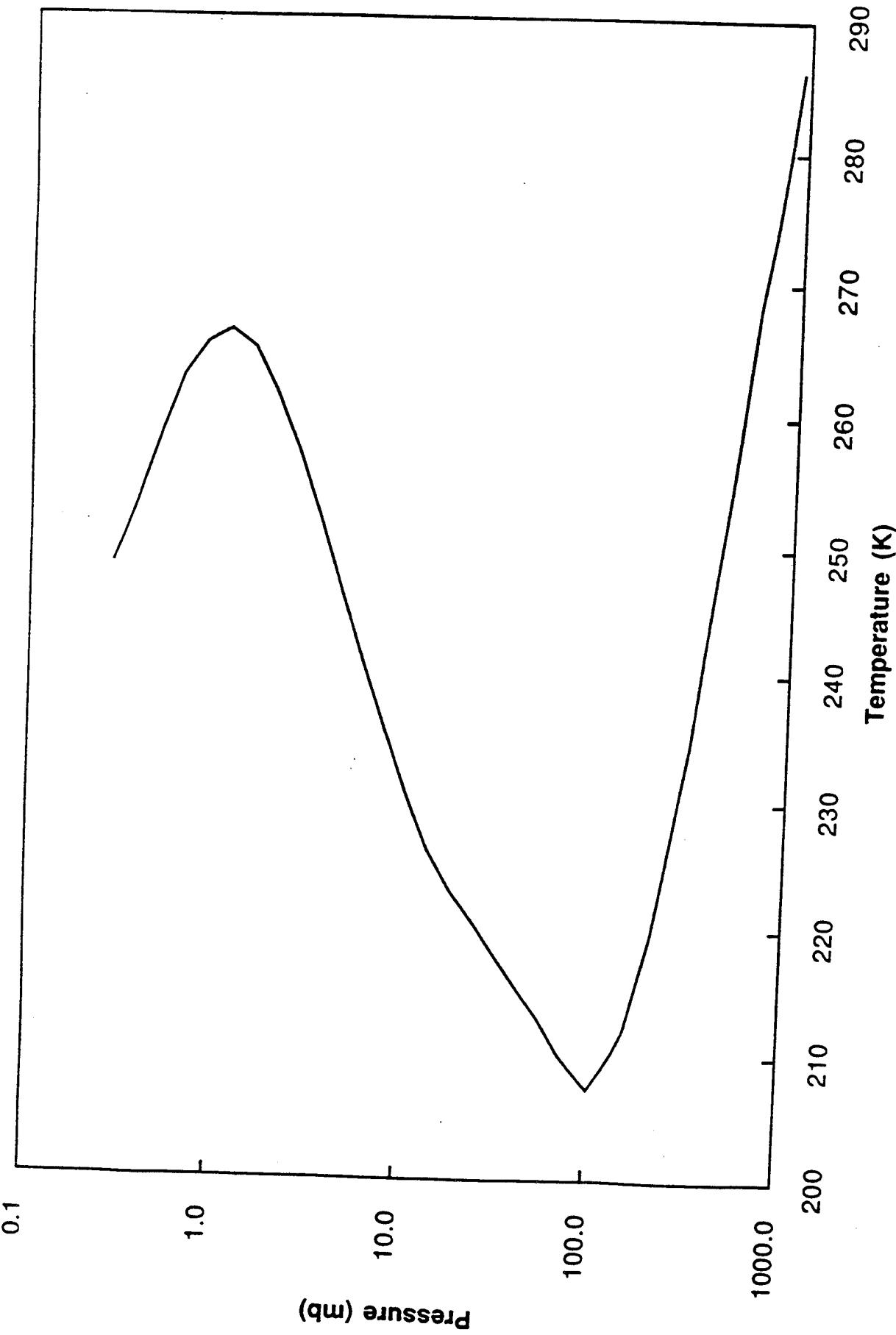
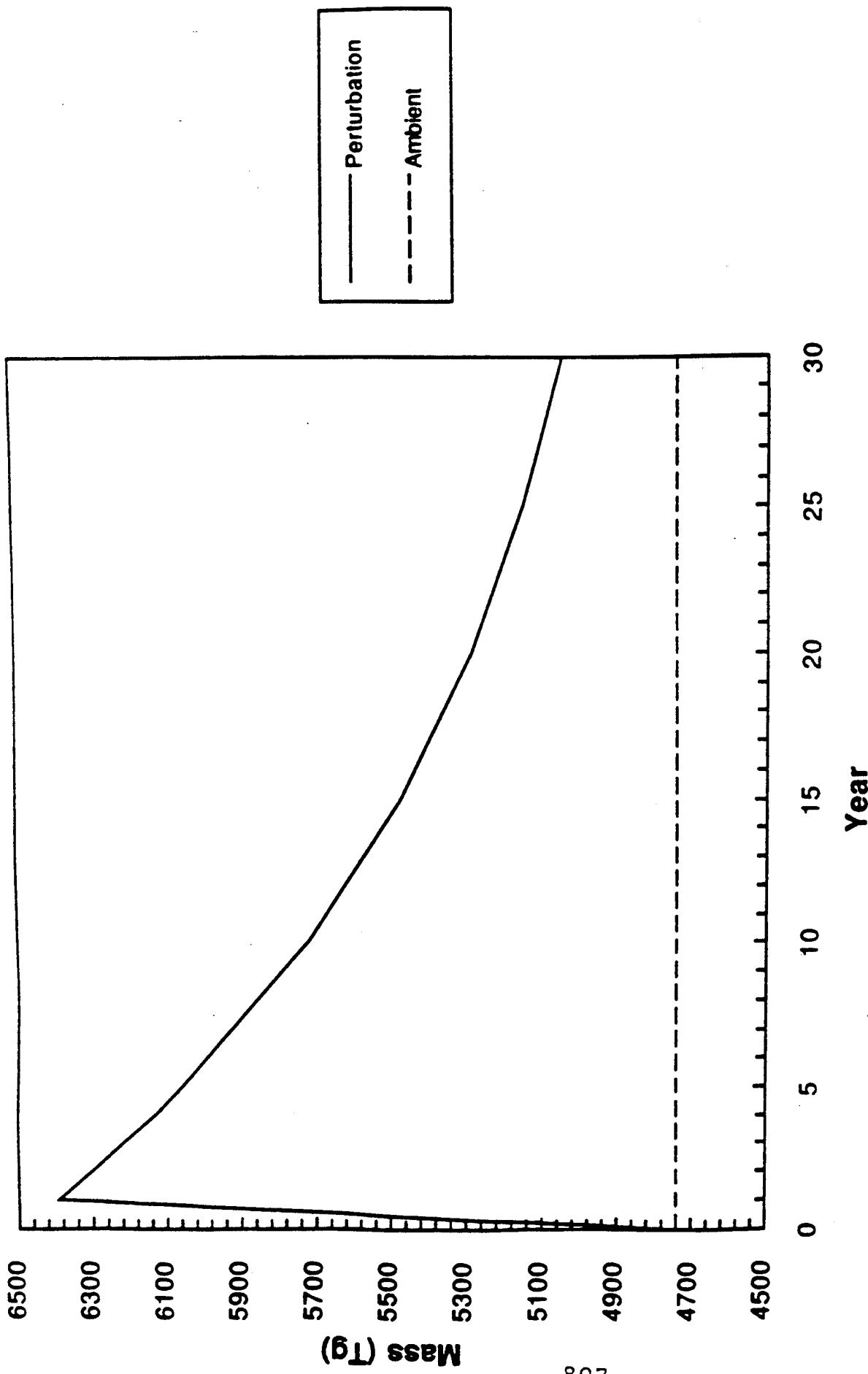


Figure 2 Pressure-temperature profile for ambient atmosphere. The temperatures are globally- and annually-averaged.



**Figure 3** Total mass of methane (in units of teragrams) in the model atmosphere as a function of time before and after a pulse emission of methane equal to the equilibrium increase of CH<sub>4</sub> produced by a constant 25% increase in total emissions. Feedbacks in the lifetime of methane result in about a 36% peak increase in total atmospheric methane. The ambient value of the methane mass is indicated by the dashed line.

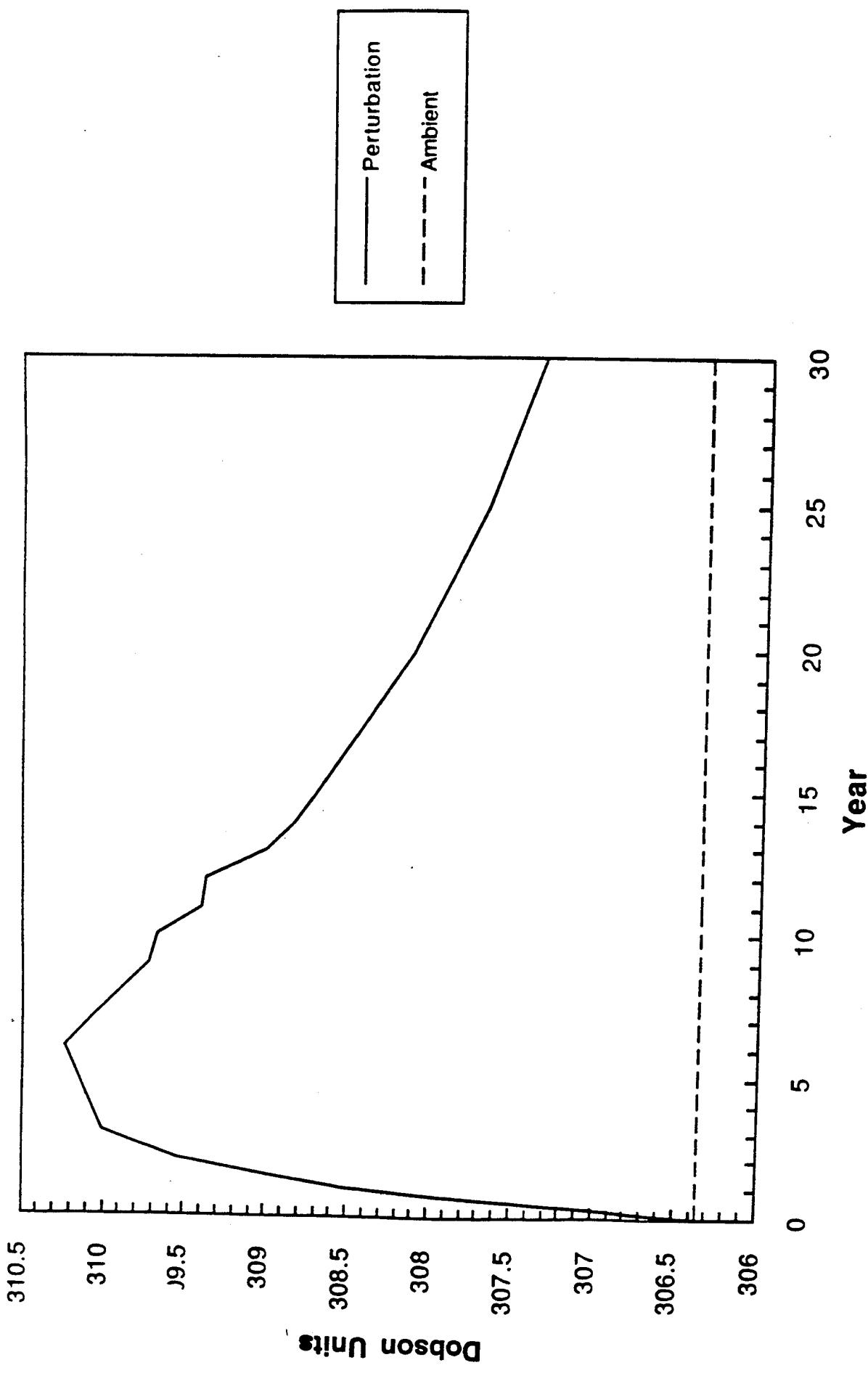


Figure 4 Annual average total ozone column after the pulse increase of methane.

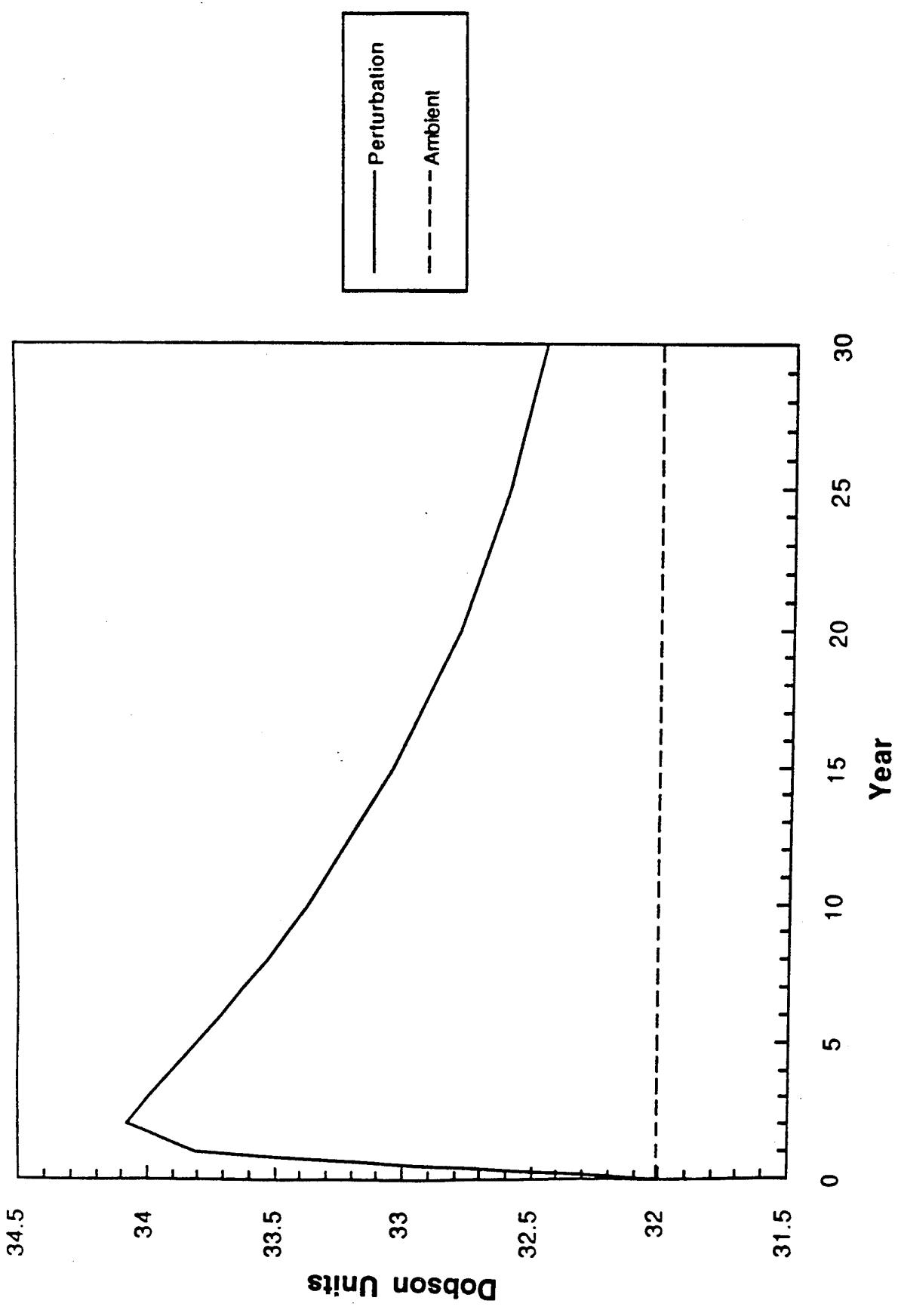
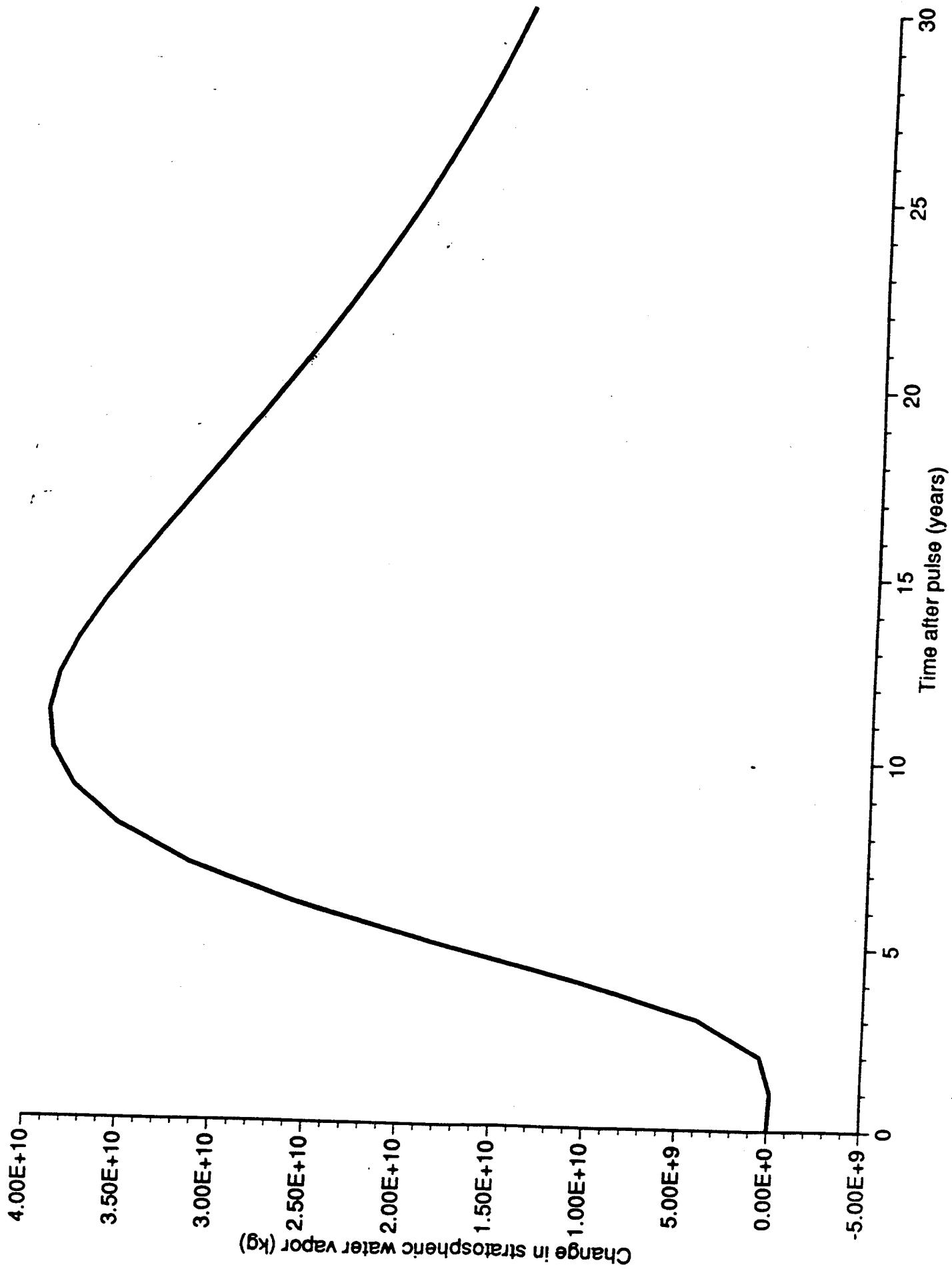


Figure 5 Annually averaged tropospheric ozone column after the pulse increase of methane.



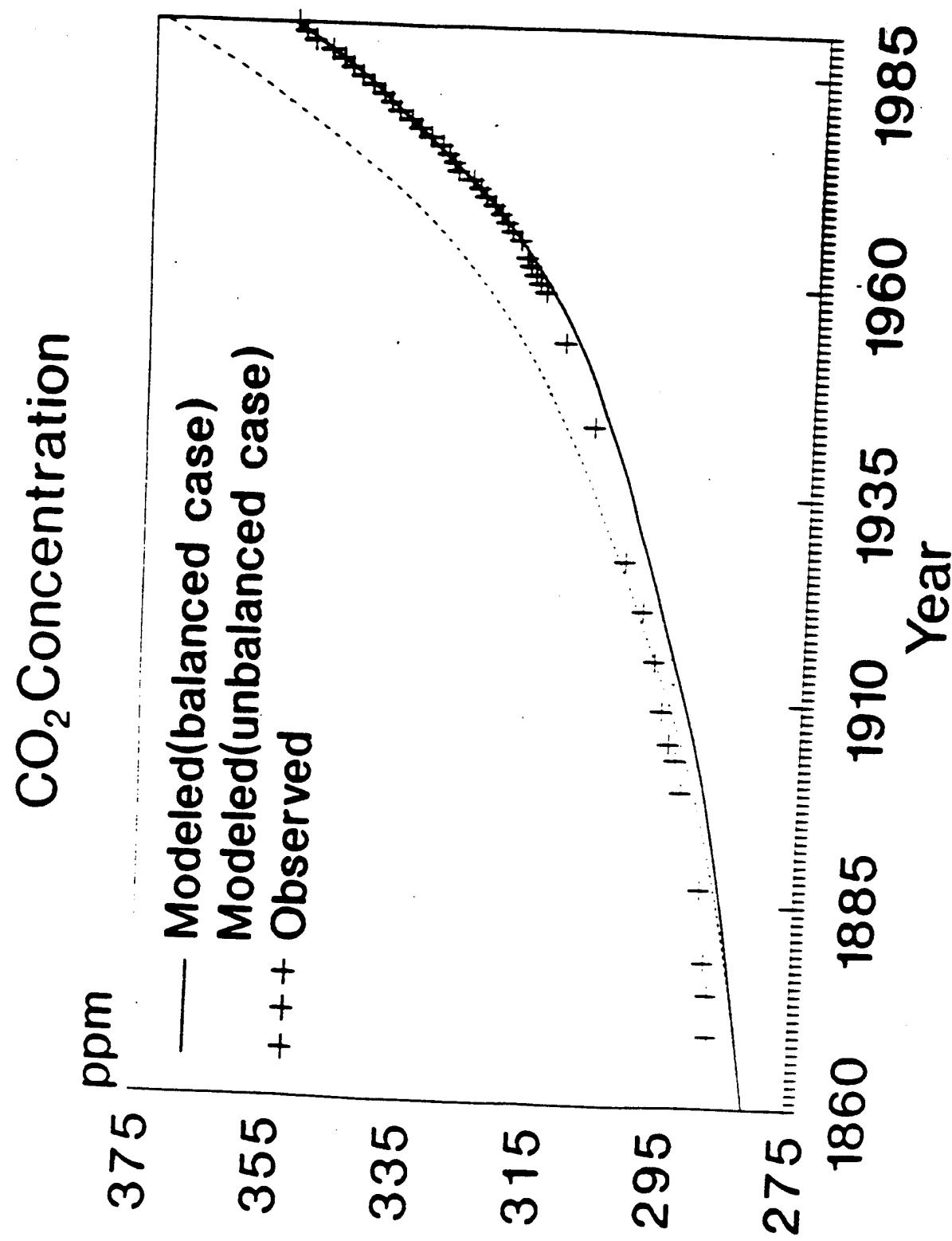
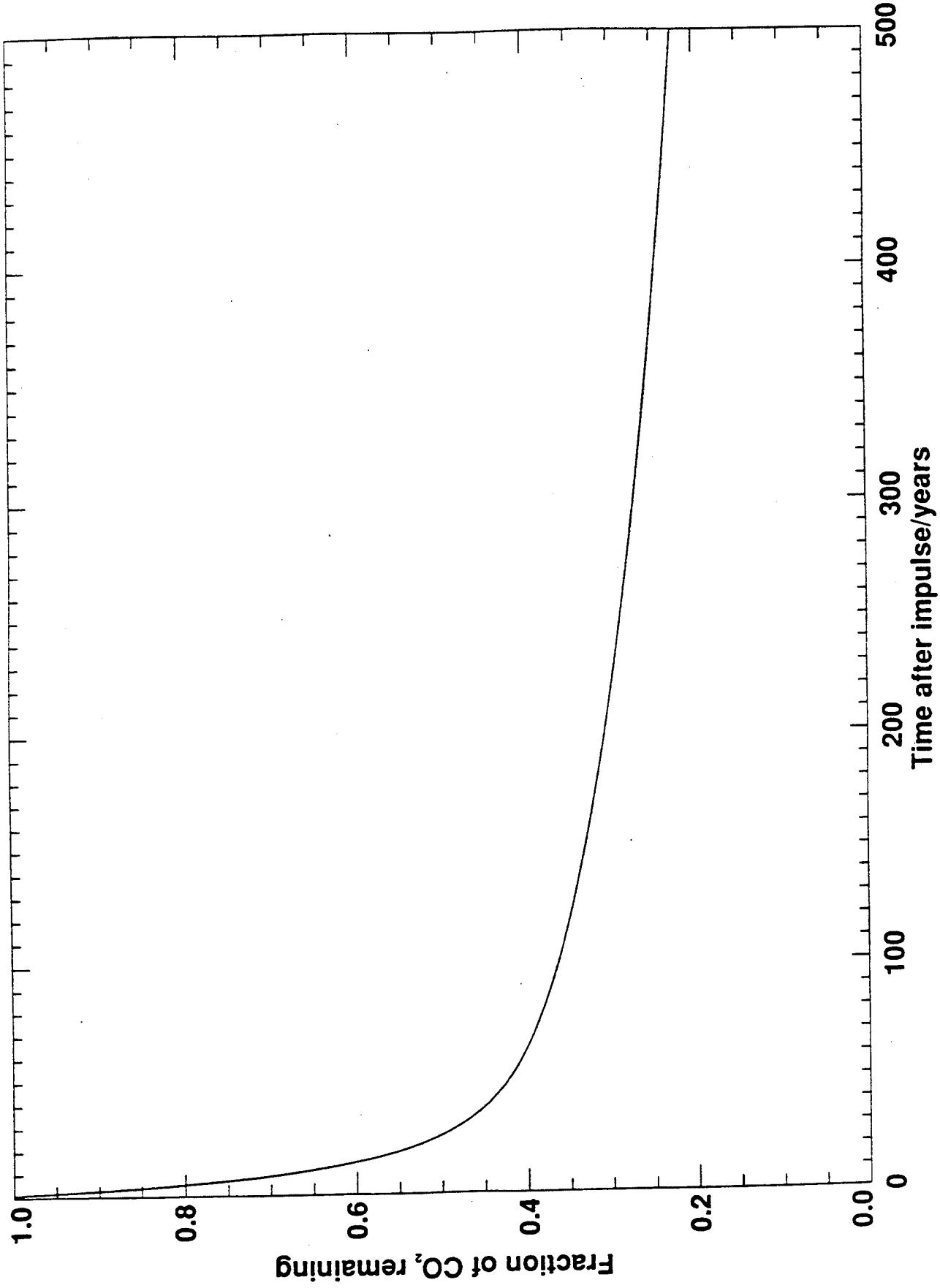


Figure 6



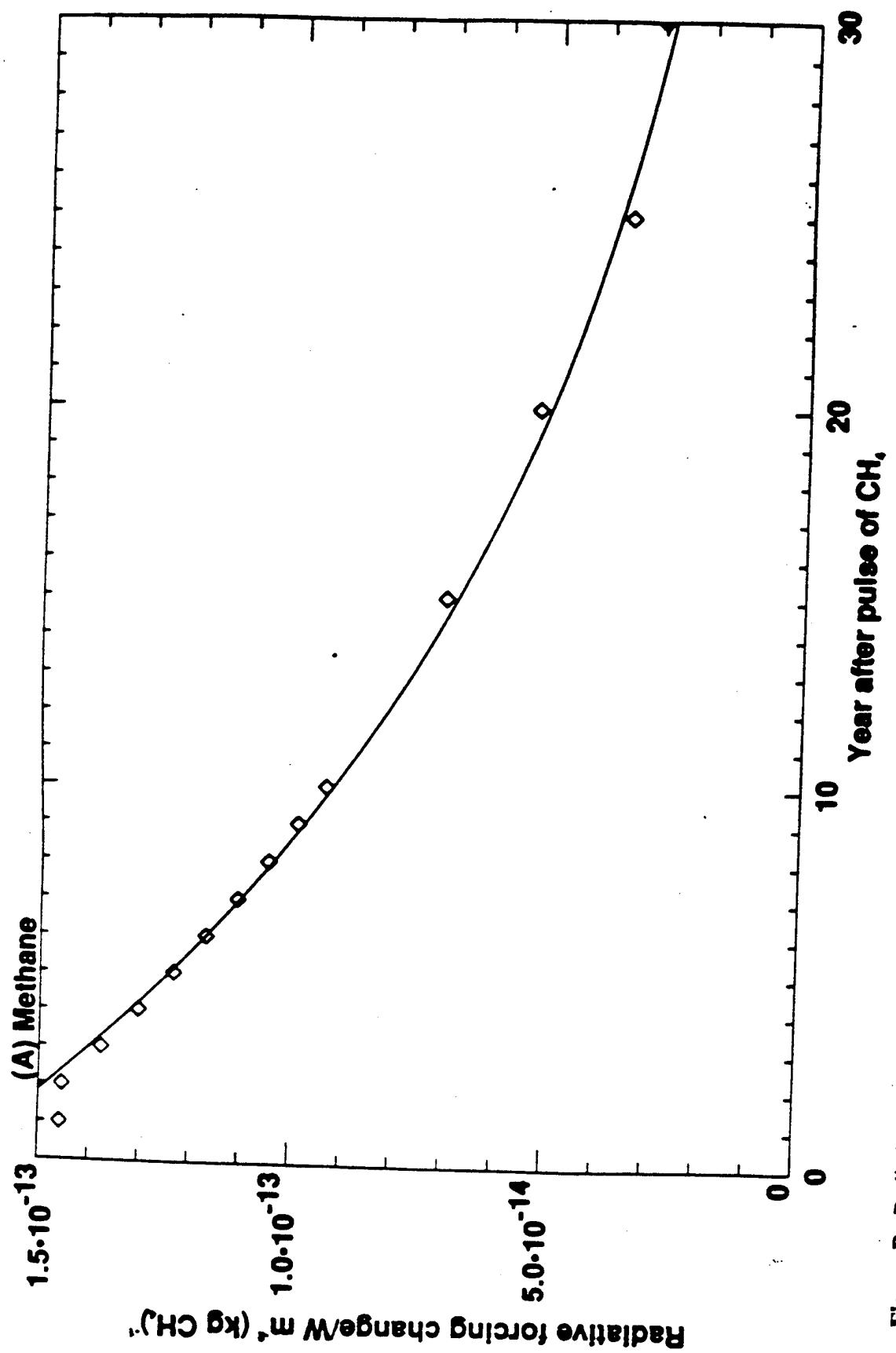


Figure B. Radiative forcing of CH<sub>4</sub> versus time after pulse release of CH<sub>4</sub>. ◊: line model calculations. Solid line: fit of Equation 5.4a.

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**17th Annual Review Conference on  
Atmospheric Radiation Models**

**ABSTRACTS**

7-8 June 1994  
PL/Geophysics Directorate  
Science Center

## **FASCODE: AN UPDATE AND RECENT VALIDATIONS/APPLICATIONS**

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FASCODE, the DoD standard line-by-line (LBL) code, has undergone only minor changes over the past two years, since the release of FASCOD3P in March 1992. Present/future capabilities and their driving requirements will be reviewed. In addition, the results of two recent comparisons of FASCODE against other LBL codes, both initiated by the WMO (World Meteorological Organization) will be presented: Intercomparison of Transmittance and Radiance Algorithms (ITRA) in the microwave region, and InterComparison of Radiation Codes used in Climate Models (ICRCCM) in the more historic infrared spectral range.

## **MODTRAN3, MODTRAN4, AND BEYOND**

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The MODTRAN code continues to be an invaluable tool for predicting and modeling radiation transport in the lower atmosphere (< 60km). The newest version, MODTRAN3, will be released shortly. Its enhancements include: (1) arbitrary layer resolution (2) improved treatments for single scatter solar and multiple scatter radiances (3) CFC, UV NO<sub>2</sub>, UV SO<sub>2</sub> and new O<sub>3</sub> Chappius cross-sections (4) a spectrally varying surface albedo input option (5) HITRAN 94 based band model data. Current research which will lead to upgrades for MODTRAN4 and later include: improved cooling rate, vertical flux, and weighting function calculations; higher spectral resolution; an updated aerosol database; vector optimization; and incorporation of the NRL climatology database via the SAG code.

## **MOSART: AN UPDATE ON THE MODERATE SPECTRAL ATMOSPHERIC RADIANCE AND TRANSMITTANCE CODE**

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The Moderate Spectral Atmospheric RTransmittance Code is currently undergoing beta testing and is scheduled for release in August 1994. Since the overview last year, a number of new capabilities have been added. These include an earthshine and skyshine model, improved classification for terrain types, and upgrades to the global terrain database and aerosol model. General verification and validation has been performed primarily with comparisons to MODTRAN, while limited direct validation has been performed with data comparisons.

## **PLEXUS**

### **PHILLIPS LABORATORY EXPERT UNIFIED SOFTWARE**

**Dr. Frank O. Clark**

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PLEXUS, or Phillips Laboratory Expert Unified Simulator, places PL Codes in a unified knowledge based interface. PLEXUS is intended for the intelligent non-expert as well as expert users. PLEXUS contains: the standard Atmospheric Generator (SAG), MODTRAN (& LOWTRAN), a validated integrated MODTRAN and SHARC pre- and post- processor combination, CBSD (Celestial Background Scene Descriptor). With a single set of input parameters from the user, the preprocessor automatically runs MODTRAN below 50 km and SHARC above 50 km and produces a single output, permitting sight paths which cross the equilibrium/non-equilibrium boundary. PLEXUS also contains the new Standard Atmospheric Generator which is based on NASA MSIS-90 and NRL lower atmosphere phenomenology data. This seamless model implementation is essential for modern space based, TMD, and GPALS applications. The single geometry interface applies to all codes.

## **EOSAEL92 UPDATE**

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Since the distribution of EOSAEL92 several of the modules have been updated and an acoustics module has been selected for incorporation. The TARGAC model has been extended and an interface to run the module under Microsoft Windows has been developed. The UVTRAN model also has a version that runs under Microsoft Windows. Both of these will be demonstrated at the conference. The millimeter wave module, NMMW, has been updated with a new gaseous absorption algorithm. The Scanning Fast Field Program (SCAFFIP) is an acoustics model that predicts acoustic propagation based on spherical spreading, molecular absorption, refraction, acoustically complex ground impedance, and diffraction over being terrain. We are in the process of making all of these modules and documentation available through the Test and Evaluation Community NETwork (TECNET). In addition the Validation and Verification of the laser transmission module, LZTRAN, has been performed.

**THE NAVY OCEANIC VERTICAL AEROSOL MODEL  
IN A FORTRAN SUBROUTINE FORMAT**

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A FORTRAN version of the Navy Oceanic Vertical Aerosol Model, NOVAM, has been completed and is ready to be interfaced with other types of transmission models. The model is available in the form of a NCCOSC RDT&E DIV technical report #1634 which contains: (a) a written description of the model, (2) the printed code of the subroutine, (3) the printed code of the associated subroutines and functions, and (4) a sample driver which can be used for batch processing of data. The model requires meteorological data in the form of both surface and atmospheric sounding data files. NOVAM predicts the vertical distribution of aerosol in the first 6 km above the ocean. Outputs of the model include optical properties in the wavelength band from 0.2 to 40 micrometers at any altitude. These properties include the volume extinction and absorption coefficient, the relative humidity, as well as parameters describing the aerosol size distribution in terms of  $dN/dr$  at that altitude. This paper will describe the model and some sample applications.

## **THE NATURE OF DESERT AEROSOLS: SUMMARY OF CHINA LAKE STUDIES TO DATE**

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**and**

**L.A. Mathews retired from  
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The Naval Air Warfare Center has been conducting desert aerosol characterization measurements at China Lake at ground level in 1987; at 15,000 feet in connection with Long Jump in 1988; at ground level in the western Mojave including Edwards AFB and China Lake in 1990; and will be conducting further measurements in the western Mojave in the summer of 1994. This presentation will present an over view of the analysis of data to date. The properties of desert aerosol that are appearing are somewhat different than those proposed by Longtin and Shettle in that the accumulation mode is dominated by the presence of large numbers of organic carbon particles while dust is characterized by the presence of clay particles in the dust size distribution mode with few quartz particles being present and no quartz dominated blowing sand mode. We will compare particle size and composition at 15,000 feet and ground level, further micrographic studies of the composition of high altitude aerosols and the effect of wind speed on aerosol characteristics at ground level.

## **APPLICATION OF THE MODTRAN2 CODE TO THE MODELING OF SILICATE DUST CLOUDS.**

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The MODTRAN2 code has been used to model the thermal infrared radiance from a dust cloud formed during an explosives test at the White Sands Missile Range in 1993. High signal-to-noise infrared spectra of the dust cloud were measured, indicating the presence of silicate particles. A silicate dust cloud was defined as part of the model atmosphere, and MODTRAN was used to calculate radiance spectra between 6 and 16 microns. A description of the analysis, comparison with experimental data, and the problems encountered will be presented.

## **MODELIZATION OF CLOUD RADIATION AND COMPARISON WITH AIRBORNE MEASUREMENTS**

**C. Malherbe, P. Simoneau and A. Boischot**

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We have developed a computer code named NUALUM, dedicated to the computation of the atmospheric radiance in presence of clouds.

This radiance is the sum of three terms:

- the atmospheric radiance between the cloud and the observator
- the thermal radiance of the cloud
- the scattering by the cloud of the solar, the terrestrial and the atmospheric fluxes.

The bidirectional reflectivity and the emissivity of the cloud are computed with the DISORT program. The solar flux, the terrestrial flux, and the atmospheric flux are calculated by MODTRAN. Numerical results are compared with spectral and spatial infrared measurements performed by airborne devices.

## **OSIC - AN ULTRAVIOLET TRANSMISSION AND MULTIPLE SCATTERING MODEL**

**Michael Neer and Kathy Crow**

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A novel analytical approach is presented for predicting not only conventional transmission associated with molecular and aerosol scatter and absorption, but also the contribution of multiple scattering including angle of arrival. The approach has been implemented in a model called MWR and sample signature versus time predictions will be presented along with comparisons to experimental data. The program will run much faster than Monte Carlo models so it is better suited to carrying out missile signature parametric studies. The model can also be used to predict signatures when the source is not in the sensor field of view and the received signal comes only from scattered radiation.

# **ATMOSPHERE UV-VISIBLE RADIATION FIELD PERTURBATIONS PRODUCED BY CLOUDS AND AEROSOLS: COMPARISON OF RESULTS USING MONTE CARLO, DISORT AND INTEGRAL EQUATION METHODS**

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The UV-Visible stratosphere radiation can be strongly perturbed from the clear atmosphere case when clouds and/or aerosols are present. The clear atmosphere is, to within ~2% accuracy, isotropic. When clouds and/or aerosols are present the radiation field can become anisotropic to a degree that isotropy is no longer a useful assumption, an inclusion of these effects is necessary either by approximation or by a more representative numerical description. We compare the results from three different approaches to the calculation of the radiation field when clouds and/or aerosols are present. Results are presented for the 280-800nm wavelength region and for a range of solar zenith angles.

We find that the integral equation solution assuming isotropic scattering is accurate to ~2% for a clear atmosphere and when similarity transformations are included, accurate to ~5-20% when aerosols and/or clouds are present, the variation in accuracy depending on wavelength, solar zenith angle, altitude and cloud or aerosol extinction optical depth. The Monte Carlo and DISORT results employ either the actual phase function calculated from a Mie scattering code, or a Henyey-Greenstein representation of the phase function.

## **INCLUSION OF ACCURATE MULTIPLE SCATTERING IN MODTRAN**

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An accurate multiple scattering scheme has been incorporated into MODTRAN by merging it with the general-purpose multiple scattering algorithm DISORT. The multiple scattering source functions for solar as well as thermal radiation are computed in DISORT and fed into MODTRAN where they are combined with the single scattering solar and thermal source terms. The complete intensity distribution is then computed in MODTRAN by integrating along the line-of-sight. The importance of this improved multiple scattering computation is demonstrated by comparing results from the original MODTRAN with those produced by the merged MODTRAN/DISORT package for radiation in the solar, thermal, and solar/thermal crossover spectral regions. In the ultraviolet/visible region the improvements are significant even for clear sky conditions, while multiple scattering effects are important in the thermal region only in the presence of clouds and aerosols. Comparisons with experimental data will also be used to demonstrate the superior performance of the merged package.

## **AN APPLICATION OF RADIATIVE TRANSFER THEORY TO UNDERSTANDING AEROSOL MTF**

**David H. Tofsted**

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Aerosol forward scattering effects can significantly blur distant objects when the Mie size parameter becomes large (such as snow, rain, fog in the visible). Starting with previous radiative transfer forward scattering approximations, we have developed a new means for determining these effects on the aerosol MTF. This derivation allows for inclusion of horizontal inhomogeneities of aerosol densities and species, uses the aerosol forward scattering approximation of radiative transfer theory, and models the aerosol phase function forward peak as a sum of Gaussian components. Using Gaussian phase function components yields an exact solution to the radiative transfer function under the forward scattering approximation. The results of the radiative transfer calculation have been translated directly into terms compatible with a linear filter interpretation of incoherent imaging. Thus the aerosol MTF derived directly from the radiative transfer analysis and does not depend on system characteristics.

## **MOLECULAR AND AEROSOL EFFECTS ON AIRBORNE LASER PROPAGATION**

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Recent missions for lasers on airborne platforms require propagation through long, horizontal, high altitude slant paths. Propagation is affected by upper tropospheric and stratospheric molecules and aerosols. Extinction coefficients and transmissions for specific high energy laser and laser radar wavelengths have been calculated using FASCOD3P/HITRAN92. The relative importance of various molecular constituents are affected because the influence of water vapor is significantly less than it is near the surface. Stratospheric aerosols can cause considerable attenuation following a major volcanic eruption. We have used NASA SAGE (Stratospheric Aerosol and Gas Experiment) satellite data to evaluate the effects of the Mount Pinatubo eruption on airborne laser propagation at certain wavelengths. We have also determined probability of occurrences of cirrus at the air-to-air mission path altitudes for different seasons.

## **GROUND-TO-SPACE ATMOSPHERIC TRANSMITTANCE MEASUREMENTS IN THE 3-5 AND 8-12 $\mu$ m SPECTRAL REGIONS: COMPARISON WITH LOWTRAN 7**

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The computer code LOWTRAN is widely and extensively used for the prediction of the propagation of IR radiation through the atmosphere. The latest version of this code, the LOWTRAN 7, is assumed to be the most elaborate and accurate one. Hence it was decided to test its validity by comparing its prediction for ground-to-space slant paths with actual transmittance measurements with the sun as a blackbody source. A good agreement between the theoretical predictions and the experimental results was obtained in the 8-12 $\mu$ m spectral region for all zenith angles between 90° and 60° (0° to 30° above the horizon). In the 3-5 $\mu$ m spectral region some spectral discrepancy was observed though the value of the integrated measured transmittance agreed well with the predicted one. The reasons for this can be assumed to be in the new band model absorption parameters (in the 3-4 $\mu$ m region) and in the water continuum model (in the 4.4-5.2 $\mu$ m region).

**WEATHER AND ATMOSPHERIC VISUALIZATION EFFECTS (WAVES)  
FOR SIMULATION**

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The WAVES suite of codes ascertains and visualizes environmental effects due to natural clouds/haze and fog. WAVES determines the illumination passing through multiple inhomogeneous cloud layers and the resulting radiance field. The effects of aerosol forward scattering and optical turbulence are also included.

## **SPARTA'S LIDAR SIMULATION CODE, BACKSCAT VERSION 4.0**

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Since 1988, SPARTA, Inc. has been developing a lidar simulation package for the IBM PC environment called BACKSCAT. The package simulates the backscatter return from lidar systems of different designs, viewing geometries, and atmospheric conditions. This paper will describe the latest version, BACKSCAT Version 4.0, and present sample results. The package will be available for distribution within a few months. BACKSCAT Version 4.0 includes many new technical features. Foremost is the ability to evaluate signal-to-noise performance for direct detection and coherent Doppler lidar systems. Signal-to-noise ratios are then used to estimate the accuracy of range and wind speed measurements for the chosen lidar configuration. These capabilities transform BACKSCAT into a more general purpose lidar simulation tool for users who want to design a lidar system to explore specific aspects of the atmosphere. In response to the user community, the second new feature is the ability to include water clouds in lidar simulations. Although the existing user-defined aerosol option could be used to represent water clouds, it required detailed cloud particle size distribution data that might not be available to some users. Thus, as an alternate approach, water clouds now can be "clicked on" automatically as a built-in cloud model. The third new feature is auxiliary software that estimates the molecular absorption profile for a particular lidar wavelength. Although previous versions of BACKSCAT provided the means to include molecule absorption in a simulation, the code did not provide a tool to calculate it. The molecular absorption package has been nicknamed MABS and generates output that can be directly used in a lidar simulation. It must be noted that the spectral resolution in MABS probably exceeds that of most lidars, so the package is not intended to be a complete treatment of the molecular absorption problem.

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## THE SOLAR IRRADIANCE BY COMPUTATION

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I am now able to compute a purely theoretical model photosphere that reproduces the irradiance measurements of Neckel and Labs in the visible for bandpasses of approximately 2 nm. That model and Avrett's empirical quiet sun model are used to predict the irradiance out to 200 microns. At 200 microns the chromosphere in the empirical model is responsible for most of the flux. Actually, monochromatic irradiance is required to determine the absorption by molecular lines in the atmosphere. I am producing atlases of the solar flux, central intensity, and limb spectra taken by James Brault at Kitt Peak. One atlas "Solar Flux Atlas from 294 to 1300 nm" by Kurucz, Furenlid, Brault, and Testerman (1984), has been published thus far. I also have the "Photometric Atlas of the Solar spectrum from 1,850 to 10,000 cm<sup>-1</sup>" by Delbouille, Roland, Brault, and Testerman (1991) also taken at Kitt Peak. In addition I have the ATMOS central intensity atlas from 650 to 4800 cm<sup>-1</sup> taken by Farmer and Norton (1989) from Spacelab 3. Parts of the flux atlases directly give the irradiance spectrum but much is confused or obscured by terrestrial lines. The intensity atlases can be used as guides for deconvolving blends because the solar lines are narrower. One path I am pursuing is fitting the transmission spectrum empirically and simply dividing it out. However, the regions where the transmission is too low, there is no alternative but to compute a purely theoretical solar spectrum. I use these atlases to test the pure calculations of solar spectra and of transmission spectra. I identify problems with the line data and I try to make generic corrections that improve hundreds or thousands of lines at a time. If the spectrum calculations look good in the regions that have high transmission are computed accurately. The main problem has been continuum placement. Ozone and O<sub>1</sub> "dimer" features are difficult to determine because the atlases are each made up of a number of sharply peaked FTS scans. The continuum placement affects the appearance of line wings and the apparent depth of weak features. To get a feel for the scope of the monochromatic irradiance problem I have computed the spectrum from 150 nm to 200 microns at a resolution of 500000 using 58 million lines, both predicted and observed. These are the same lines that went into computing the opacity for the model photosphere. If this spectrum is degraded to the resolution of the model it looks like the model. At any given monochromatic point the spectrum is not reliable. But at a resolution of 10000, say, it approaches measurement accuracy. In regions of low transmission it is more reliable than existing measurements. I will publish tables of these irradiance spectra at various resolutions.

**NEW VISIBLE AND NEAR IR OZONE ABSORPTION CROSS-SECTIONS  
FOR MODTRAN**

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Knowledge of the ozone absorption cross-sections is important for modeling the propagation of radiation through the atmosphere, and is critical for deriving the atmospheric ozone concentration from measurements of the spectral character of transmitted or scattered radiation. While the ultraviolet cross-sections for ozone were completely replaced in LOWTRAN 7, the visible cross-sections are unchanged since the original version of LOWTRAN and the cross-sections are not given at all for wavelengths longer than 769 nm. Recently there have been several new spectroscopic studies of the ozone Chappuis and Wulf absorption bands, along with measurements of the absolute cross-section at selected wavelengths. We have normalized the spectral measurements to the absolute cross-section data, and smoothly joined the different sets of measurements, to provide the ozone cross-section from 407 to 1089 nm. The temperature dependence is also given for 407 to 762 nm. It is anticipated that these cross-sections will be included in MODTRAN 3.

## **ABSORPTION CROSS SECTION MEASUREMENTS OF CARBON DIOXIDE IN THE WAVELENGTH REGION 118.7-175.5 nm AND THE TEMPERATURE DEPENDENCE**

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In absorption, CO<sub>2</sub> is transparent down to at least 210 nm. Photoabsorption cross section measurements of CO<sub>2</sub> in the UV to VUV region have been made by several investigators. Because of lack of resolution, none of the studies in the period 1950-70 resolved the structures in the CO<sub>2</sub> absorption cross sections. After investigating photographic plates of CO<sub>2</sub> absorption spectra taken in high resolution, we confirmed that structures in the CO<sub>2</sub> are broad enough to allow the use of a medium resolution instrument. The 3-m spectrometer on the BL-20A beam line at the Photon factory, Japan was used in the first order of a 1200 l/mm grating to obtain absorption cross sections of CO<sub>2</sub>. The background continuum is provided by the synchrotron radiation source without any order separation, because any high order radiation is cut off by MgF<sub>2</sub> windows. The absorption cross sections of CO<sub>2</sub> were obtained at two temperatures, 195 K and 295 K, in the wavelength region 120-175 nm for every 0.005 nm step. Almost no temperature dependency was observed in the peak cross sections in the wavelength region 125-143 nm, however, the ratio of peak cross sections are down to 0.7 around 175 nm. This work is supported by NASA Upper Atmospheric Research Program under the Grant No. NAGS-494 to the Smithsonian Astrophysical Observatory.

## FASCODE ENVIRONMENT (FASE)

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The Optical Physics Division of the Phillips Lab is developing a state-of-the-art line-by-line atmospheric transmittance/radiance model as the successor to FASCODE. Under a joint program with DoE's Atmospheric Radiation Measurement (ARM) project, the best features of FASCODE and the DoE's standard radiative transfer program **LBLRTM** will be merged and new capabilities developed. While retaining all of FASCODE's capabilities, FASE will specifically address environmental applications such as atmospheric heating rates and temperature and species inversion.

The main features of FASE will be:

- Highly modular all the basic function--l-b-l optical depth, radiative transfer, atmospheric profile, filtering, scanning and plotting--will be broken out into independent programs These program can be run together through a driver just as FASCODE is now, run separately, or incorporated into customized applications: e.g., multiple scattering codes or inversion routines
- Core module: line-by-line calculation of optical depth: incorporate best Physics: including continua, line coupling, cross-sections of heavy molecules.
- Optimized: for vectorized and/or parallel processing
- Interface: improved user-friendliness
- Improved packaging: makefile for easy installation on a wide variety of platforms.
- Configuration controlled: for ease of maintenance

## **SSGM: THE STRATEGIC SCENE GENERATION MODEL**

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The Strategic Scene Generation Model generates viewer-perspective pixel apparent radiance maps and point-source intensity data. These scenes are computed from the output of state-of-the-science phenomenology codes and their authenticated input databases. Scenes consist of quiescent and enhanced natural and perturbed backgrounds with embedded targets and target related events. Backgrounds include terrain, clouds, earthlimb, space, aurora, horizon, and nuclear events. Targets include boosting missile plumes and hardbodies, fuel vents, and post-boost objects including RV and decoys. A review of the robust Earthlimb Capabilities in Release 6.0 will be presented.

## LIDAR MEASUREMENTS OF ATMOSPHERIC OPTICAL PROPERTIES

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The LAMP (Lidar Atmospheric Measurements Program) lidar instrument has been used to develop and refine techniques for measurements of atmospheric properties. The initial measurements primarily focused on the measurement of middle atmosphere dynamics and structure. More recent efforts have concentrated on measurements of tropospheric water vapor and temperature. The vibrational and rotational Raman scatter signals used for these lower atmospheric profiles can also be used to determine the backscatter and extinction profiles. The optical extinction profiles determined from the Raman scatter signals at several wavelengths provide a measure of the wavelength dependence of aerosol and cloud layers in the troposphere. Several examples of the optical extinction profiles have been examined and comparisons with inversion techniques from the backscatter have shown limitations of the inversion analysis. The inversion of backscatter profiles does not generally yield satisfactory results. These investigations show that the Raman lidar measurements provide a most useful way to measure the atmospheric optical properties.

## **GROUND-BASED MEASUREMENTS OF HF AND HCI**

**Hilary E. Snell and Paul B. Hays**  
**University of Michigan**

This poster describes remote sensing observations of HF and HCI column densities over Ann Arbor, Michigan. Spectra were collected between October 1992 and July 1993 using a ground-based Michelson Interferometer and the technique of solar absorption spectroscopy. While the column densities computed from these spectra agree with other groups' measurements of these species, we have noticed that the HCI spectral line at  $2925.897 \text{ cm}^{-1}$  appears strongly asymmetric. It is our belief that this is due to spectral contamination by another chemical species and not instrumental phase errors as previously reported by other groups.

**AN ATMOSPHERIC MODEL FOR GRAVITY WAVE INDUCED TURBULENT LAYERS  
(BLINI) BASES ON THE SATURATED CASCADE MODEL**

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Turbulence in the atmosphere above the boundary layer occurs in thin, pancake-shaped horizontal layer called "blini". These are generated by gravity waves whenever the Richardson number is less than a critical value. A theory which seems to accurately predict atmospheric gravity wave spectra was recently published in GRL (Dewan, May 1, 1994, vol. 21, p.817). This theory also implies wave number-period relationships used below. On the basis of this theory, simulations were made of gravity wave fields by means of a superposition of random (phase and amplitude) sine waves consistent with the vertical wave number spectrum of horizontal wind fluctuations. Whenever shears exceeded critical values, the computer program graphed the locations on an altitude-plot. As a result, realistic blini appear which, as was anticipated, "blink" on and off. Subsequently this model will go by the name "The blinking blini model for atmospheric turbulence". It will be used, in the future, together with laser propagation codes to ascertain the effects of wave induced turbulence on ABL systems.

## **PRELIMINARY RESULTS FROM A RECENT ICRCCM INITIATIVE**

**F. Miskolczi, M. Bonzagni, R. Guzzi**  
**University of Maryland**

In this paper high resolution measured and computed atmospheric downward radiance spectra are compared. The spectral measurements were taken during the SPECTRE experiment (Coffeyville, Kansas 1991) using the UWI AERI fourier spectrometer. The radiance modeling is based on the High-Resolution Atmospheric Radiance-Transmittance Code (HARTCODE) (F. Miskolczi, M. Bonzagni and R. Guzzi, 1990). In this comparison the seven major absorbers, F11, F12, N2 and CCL4 were included.

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Reference:

F. MISKOLCZI, M. BONZAGNI, R. GUZZI (1990)  
High Resolution Atmospheric Radiance-Transmittance Code (HARTCODE).  
Meteorology and Environmental Sciences, World Scientific  
Pub. Co., 1990, pp. 743-790

## **STRUCTURE IN RADIATIVE EXCITATION AS A SOURCE OF HIGH ALTITUDE RADIANCE STRUCTURE: CO( $v=1$ ) RADIANCE**

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We discuss a largely overlooked source of upper atmosphere structured radiance, structure in the earthshine pumping rate caused by a structured lower boundary. The 4.7  $\mu\text{m}$  radiance from CO( $v=1$ ) is a good example of a non-LTE emission that is dominated by radiative processes. The analysis of limb spectra of both the  $^{12}\text{C}^{16}\text{O}$  and  $^{13}\text{C}^{16}\text{O}$  from CIRRIS 1A data (Dodd et al., GRL, 20, 2683, 1993) clearly indicated how the differing opacity of the isotopes controlled the effect of pumping from the lower boundary. We examine some limiting cases that show that nighttime earthlimb radiance variations of factors greater than 2 can be caused by cold clouds at the tropical tropopause.

## INFRARED RADIANCE FLUCTUATIONS IN THE UPPER ATMOSPHERE

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Simulation of infrared radiance fluctuations in the atmosphere depends on detailed descriptions of fluctuations in atmospheric species number densities, vibrational state populations, and the kinetic temperatures along the sensor line-of-sight. In the upper atmosphere, where nonequilibrium effects (LTNE) become important, a small fluctuation in the kinetic temperature can result in correlated, anti-correlated, or no change in the vibrational temperature of states. The relationship between kinetic and vibrational temperature fluctuations depends on the subtle interplay between changes in the total number densities, changes in the temperature-dependent kinetic rates, and the relative contribution of the radiative relaxation. The model developed in this paper predicts the two-dimensional radiance covariance function for LTNE conditions. The radiance statistics are non-stationary and are explicitly bandpass and sensor FOV dependent. The SHARC model is used to calculate mean LOS radiance values and radiance derivatives which are necessary to determine the radiance statistics. Inputs to the model include the statistical parameters of a non-stationary atmospheric temperature fluctuation model and an atmospheric profile. The radiance statistics are used in a simple model for synthesizing images. The model has been applied to calculate the radiance structure for the OH( $\Delta v=1$ ) swir band and the CO<sub>2</sub>(v<sub>3</sub>) MWIR band under nighttime conditions.

**SYNTHETIC 3-D ATMOSPHERIC TEMPERATURE STRUCTURE:  
A MODEL FOR KNOWN GEOPHYSICAL POWER SPECTRA USING  
A HYBRID AUTOREGRESSION AND FOURIER TECHNIQUE**

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Within a defined domain, geophysical phenomena often are characterized by smooth continuous power spectral densities having a negative power law slope dependence. Frequently, Fourier transform analysis has been employed to generate synthetic scenes from pseudorandom arrays by passing the stochastic data through a Fourier filter having a desired correlation structure and power spectral dependency. This report examines the possibility of producing synthetic structure by invoking autoregression analysis in conjunction with the Fourier method. Since computations that apply multidimensional fast Fourier transforms to large data arrays consume enormous resources and time, the goal of this study is to seek an alternative method to reduce the computational burden. Future editions of the Phillips Laboratory Atmospheric Radiance Codes will feature an ability to calculate structured radiance. The methods explored herein provide a process that can complement or in some cases supplement methods presently being used. Line of sight computations using the three-dimensional database will be presented.

## **PLANE WAVE SCINTILLATION IN AN ONION SKIN MODEL**

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The geometry of an onion skin model for atmospheric optical turbulence is presented for application to near horizontal propagation. This is then used to derive analytic expressions for the log amplitude variance of a plane wave in the weak turbulence (Rytov) framework. The geometrical effects on the altitude weighting function are investigated and used to define the limit of validity of the flat earth model. The formalism is then extended to include the effects of aperture averaging and non-zero inner scale. It is found that Rytov theory should be applicable to zenith angles of less than approximately 85°. It is also established that inner scale and aperture averaging are much less important for near horizontal than for vertical propagation in the weak turbulence case. Predictions of log amplitude variance are presented for calculations using the CLEAR t model as well as individual Cn2 profiles derived from balloon measurements. This formalism is readily extended to provide analytic expressions for other turbulence effects.

## **COMPARISON OF A MODEL DESCRIBING PROPAGATION THROUGH OPTICAL TURBULENCE (PROTURB) WITH FIELD DATA**

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The PROTURB model, developed by the Battlefield Environment Directorate of Army Research Laboratory, calculates an estimate of optical turbulence strength and its effects on visible and infrared imaging and laser system performance. The PROTURB model was compared to data supplied by the Army Test and Evaluation Command Ft. Belvoir Meteorological Team. Here we present a comparison using data from three locations that differ greatly in meteorological conditions and in site characteristics. We discuss the data collection and reduction effort, and show how this data compares with PROTURB predictions.

## **THE ROLE OF TURBULENCE IN CLOUD DROPLET FORMATION AND OUTSIDE CLOUDS**

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Turbulence, it is becoming increasingly clear, contains organized structures which carry fluid from one place to another through the turbulent medium. Much of the atmosphere is in a stable stratified state. In these conditions two dimensional vortices form, and smaller swirls can coalesce to feed larger scale motion. The Red Spot on Jupiter appears to be such a structure. In clouds, cooled parcels near cloud tops generate descending spherical vortices which carry diluted cloud parcels deep into the cloud. This phenomena drives the microphysical development in both cumulus and stratus clouds, and hence controls the droplet spectra and the distribution of ice, which in turn plays a large role in the radiative characteristics of the cloud. It seems likely that the mammatus protruding into the clear air below shelf clouds are of this form of motion.

## **SHARC-3: A MODEL FOR INFRARED ATMOSPHERIC RADIANCE AT HIGH ALTITUDES**

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SHARC-3 is the latest version of Strategic High Altitude Radiance Code. This talk describes new SHARC features like its ability to simulate changing atmospheric conditions along the line-of-sight (LOS) paths being calculated. SHARC has been developed by the Air Force to meet systems requirements for a simulation code that is both suitable for systems studies and which provides: rapid and accurate calculations of upper atmospheric IR radiance and transmittance spectra; has a spectral resolution of better than 1 cm<sup>-1</sup>; spans the 2 to 40 μm (250 to 5,000 cm<sup>-1</sup>) wavelength region; and accommodates arbitrary lines of sight in the 50-300 km altitude regime. SHARC accounts for the production, loss, and energy transfer processes among the molecular vibrational states important to this spectral region. Auroral production and excitation of CO<sub>2</sub>, NO, and NO<sup>+</sup> are included in addition to quiescent atmospheric processes. Calculated vibrational temperatures are found to be similar to results from other non-LTE codes, and SHARC's equivalent-width spectral algorithm provides very good agreement with much more time-consuming "exact" line-by-line methods. Calculations and data comparisons illustrating the features of SHARC-3 are presented.

## **NON-LTE IN CO<sub>2</sub> IN THE MIDDLE ATMOSPHERE**

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A new line-by-line ALI (accelerated lambda iteration) technique, initially designed to solve multilevel non-LTE line formation problem in stellar atmospheres, is applied to study effects of the non-LTE on the populations, source functions and limb radiances in various infrared CO<sub>2</sub> bands in Earth's middle atmosphere. Approximations used in previous studies of non-LTE in CO<sub>2</sub> are analyzed. Implications for remote sensing with high spectral resolution instruments are discussed.

## **COMPARISON OF LINE-BY-LINE AND MODIFIED CURTIS MATRIX NARROW-BAND MODEL APPROACHES TO RADIATIVE TRANSFER IN THE CO<sub>2</sub> 15 μm BANDS**

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We have undertaken a detailed comparison of two different models for calculating non-LTE populations in the terrestrial atmosphere, for the purpose of studying the effects of the radiative transfer algorithms that are embodied in them. The models are the iterative line-by-line RAD model that forms the basis of the PL ARC code and the inverse modified Curtis matrix (MCM) model, developed by Lopez-Puertas and co-workers. They have been used to calculate the vibrational temperatures and cooling rates in the CO<sub>2</sub> 15 μm bands. The comparison covers the altitude range 40-160 km, includes strong and weak bands, uses model atmospheres having extreme temperature structures, and also tests the effect of changing kinetic parameters. The models' vibrational temperatures and cooling rates generally agree to within 2 K and 0.5 K/day, respectively. We will show these results, discuss those aspects of the radiative transfer algorithms responsible for the small differences that do appear, and mention the implications for non-LTE code validation.

## **SUBTHERMAL NO( $^2\Pi_\Omega$ ) SPIN-ORBIT DISTRIBUTIONS IN THE THERMOSPHERE**

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The populations in the two NO( $X^2\Pi, v=1, \Omega=1/2, 3/2$ ) spin-orbit manifolds in the Earth's thermosphere have been found to depart by as much as a factor of two from the ratio expected from thermal equilibrium. The effective temperature describing the observed population distribution is hundreds of degrees Kelvin lower than the kinetic or rotational temperatures. Absolute spin-orbit specific column densities of NO( $v=1$ ) were derived from high-resolution ( $1 \text{ cm}^{-1}$ ) IR earthlimb spectra in the 100 to 200-km region, obtained in the CIRRIS 1A Space Shuttle experiment. Nonlinear least-squares synthetic spectral fitting was used to analyze the NO  $\Delta v=1$  fundamental band emissions near  $5.3\mu\text{m}$ . The spin-orbit distribution represents a third degree of freedom, along with vibration and rotation, that is not in equilibrium with the local kinetic temperature. These observations may significantly impact the remote sensing of NO in the upper atmosphere. The subthermal distribution is most likely produced in the collisional uppumping of NO( $v=0$ ) by O atoms, which is the major source of NO( $v=1$ ) in the thermosphere. Thus, spin-orbit distribution measurements may provide a means of distinguishing NO produced by chemical reaction from NO excited by collisional uppumping.

This work was supported by the Air Force Office of Scientific Research and the Ballistic Missile Defense Organization.

**COMPARISON OF GLOBAL VARIATION OF THE RADIANCE OF THE STRATOSPHERIC O<sub>3</sub>, CH<sub>4</sub> SPECTRA AS VIEWED CIRRIS 1A FORM DISCOVERY-103 WITH CLAES EXPERIMENT ON BOARD OF UARS**

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We report on measurements of these species by the Cryogenic Infrared Radiation Instrumentation for shuttle (CIRRIS 1A) which flew aboard the Discovery OV-103, STS-39 on April 28 to May 6, 1991. By looking in the limb, it was possible to obtain approximately a thousand interferograms. This made possible a certain identification of many important stratospheric gases, including O<sub>3</sub>, CH<sub>4</sub>, HNO<sub>3</sub>, and chlorine source species CCL<sub>2</sub>F<sub>2</sub>, and CCL<sub>3</sub>F. The accuracy of the CIRRIS 1A measurements is therefore of interest in polar ozone depletion studies, and validation is a major consideration. This paper will review the CIRRIS 1A observations of O<sub>3</sub>, CH<sub>4</sub>, and HNO<sub>3</sub> spectra and of vertical profiles concentration and discuss their accuracy and precision. We will compare the CIRRIS 1A measurements with the Cryogenic Limb Array Etalon Spectrometer (CLAES) on board the Upper Atmosphere Research Satellite. Specifically we will compare CIRRIS 1A and CLAES spectra in the wavelength regions targeted for O<sub>3</sub>, CH<sub>4</sub>, and HNO<sub>3</sub> concentration retrievals, and we will compare the retrieved quantities for species in the southern and northern hemispheres. Since CIRRIS 1A data were collected shortly before, and CLAES data shortly after, the Pinatubo eruption, such comparisons are of significant value both scientifically and from a validation standpoint.

## **THE POAM EXPERIMENT AND EARLY MEASUREMENT RESULTS**

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**and the POAM II Science Team**

NRL's Polar Ozone and Aerosol Measurement (POAM II) instrument was developed to measure the distribution of atmospheric aerosols, PSC's, and several molecular species critical for understanding ozone chemistry in the polar stratosphere. It was launched on France's SPOT 3 satellite on 25 September 1993. It makes solar occultation measurements in nine narrow-band channels from the visible to the near IR. From the measured transmissions, it is possible to determine the densities of aerosols at altitudes of 10-40 km, ozone at altitudes of 10-60 km, water vapor at altitudes of 15 -40 km, and nitrogen dioxide at altitudes of 20-40 km. The SPOT 3 satellite is in a 98° inclined sun-synchronous orbit at an altitude of 833 km. This results in all the POAM II measurements being in the Polar regions. We will discuss the POAM II instrument design, the retrieval algorithm, and the preliminary results of the measurements, including early data validation studies. POAM II is sponsored by the Innovative Science and Technology Office of BMDO (BMDO/DTI) and the DoD Space Test Program (STP).

## LARGE-SCALE RETRIEVAL OF ATMOSPHERIC PARAMETER PROFILES

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We have developed and tested SEASCRAPE (Sequential Evaluation Algorithm for Simultaneous and Concurrent Retrieval of Atmospheric Parameter Estimates), a code designed to automate and expedite the retrieval of atmospheric profiles from large quantities of remote sensing data generated by nadir and limb soundings. Our algorithm uses a *sequential* parameter estimation method known as the Square Root Information Filter, a numerical technique for solving least squares problems that is particularly suited for handling large volumes of data. The algorithm permits *simultaneous* retrieval of many atmospheric profiles. By implementing the algorithm in a parallel processing environment, *concurrent* data analysis will achieve a dramatic increase in the rate at which the data can be processed.

## **GENERAL INVERSION PACKAGE FOR RETRIEVAL OF ATMOSPHERIC SPECIES FROM HIGH RESOLUTION SPECTRAL MEASUREMENTS**

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A general inversion algorithm based on the Rodgers (1976, 1990) optimal inversion approach is being developed. The algorithm is applicable to the simultaneous retrieval of any ensemble of selected molecular species as well as atmospheric temperature from down-looking, up-looking or limb measurements. The algorithm has been designed to use FASCODE for the molecular optical depths calculations but can be modified to run with faster transmittance models (e.g. MODTRAN). Substantial computational gain is achieved over the existing "Path Characterization" algorithm (Isaacs et al. 1990), by performing the K-matrix calculation analytically and by making the code fully vectorizable. The algorithm has been applied successfully to the simultaneous retrieval of temperature and water vapor from the ground based interferometric measurements (Theriault et al. 1993). The algorithm will be applied to CIRRIS data and to MSX data when available.

## SIMULATION OF STELLAR OCCULTATION MEASUREMENTS

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An instrument for monitoring stratospheric ozone, GOMOS (Global Ozone Monitoring by Occultation of Stars), will be launched by ESA on the ENVISAT-1 satellite in 1998. The instrument measures atmospheric UV-visible transmission spectra in 250 - 675 nm at a resolution of 0.6 nm. Absorption spectra of O<sub>2</sub> and H<sub>2</sub>O are detected by two IR channels of spectral resolution 0.12 nm located around 760 and 930 nm. Transmission along slant paths of tangent heights down to 15 km is measured. Solar light scattered into the instrument FOV forms a background signal. Simulation of both the transmittance and the scattered background are required in developing the instrument and data analysis methods. Special requirements of occultation measurements are the modeling of scintillations and refractive attenuation of light (dilution of the flux density due to the decreasing of refractive index with altitude). In the case of GOMOS absorption by minor species, such as NO<sub>2</sub>, NO<sub>3</sub>, BrO, and OCIO, should also be simulated.

**LINE-BY-LINE CALCULATIONS OF ATMOSPHERIC FLUXES AND COOLING  
RATES II: APPLICATION TO CARBON DIOXIDE, OZONE, METHANE, NITROUS  
OXIDE, AND THE HALOCARBONS**

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Determining the spectral contribution of atmospheric molecular components to the total longwave fluxes and cooling rates is a necessary step toward understanding the effect and response of these gases to global climate change. Clear-sky longwave computations using a line-by-line radiative transfer model (LBTRTM) have been completed for several atmospheric profiles. We have previously presented results for both water vapor [Clough et al., 1992] and the water vapor continuum [Clough et al., 1989]. In the current paper we present the effects of carbon dioxide, ozone, methane, nitrous oxide and the most important halocarbons in addition to water vapor. Both the spectral and spectrally integrated flux and cooling rate contributions from each of these significant greenhouse gases are evaluated. Carbon dioxide, an extremely strong atmospheric absorber, is generally saturated in the troposphere with the exception of two narrow spectral bands with the result that carbon dioxide plays an anomalously small role in this altitude regime. Additional studies include the effect on the longwave cooling rates and fluxes due to the anticipated ten year changes in C02, 03, CFC-II, CFC-12, GFC-22, and CCL4 from 1990 to 2000 as well as due to the doubling of carbon dioxide

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**VERY NARROW BAND MODEL CALCULATIONS OF  
ATMOSPHERIC FLUXES AND COOLING RATES  
USING THE MODTRAN CODE**

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Because of the large computational speed advantage afforded by band models over line-by-line (LBL) models the development and application of band models to the calculation of atmospheric radiative fluxes and cooling rates continues to be an active area of research. A wide variety of narrow band model (NBM) and wide band model (WBM) approaches have been developed. Typically the calculation of spectral resolution,  $\Delta w$ , of the NBMs falls within the  $5 \leq \Delta w \leq 20 \text{ cm}^{-1}$  range, while for the WBMs  $\Delta w \geq 100 \text{ cm}^{-1}$ . Direct application of these band models to the calculation of atmospheric fluxes and cooling rates usually results in poor to only fair agreement with LBL calculations. In order to circumvent this problem the band models are treated as parameterizations rather than as first principles models. These tuned band models can yield atmospheric flux and cooling rate predictions of LBL-like quality. This paper discusses a new first principles based very narrow band model (VNBM) approach with  $\Delta w = 1 \text{ cm}^{-1}$  which yields atmospheric flux and cooling rate predictions of near LBL quality. The VNBM is incorporated in the Phillips Laboratory MODTRAN atmospheric transmittance-radiance code which enables general specification of the atmospheric species, concentration and thermodynamic profiles, calculational spectral interval, and path geometry. The relatively high spectral resolution of this approach combined with separation of the transmittance algorithm into truncated line and line wing components treats the problem of line correlation in a physically realistic manner. In order to evaluate the VNBM approach comparison is made to LBL benchmark atmospheric flux and cooling rate calculations.

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## GREENHOUSE GAS CONCENTRATION PROFILES RETRIEVED FROM CIRRUS 1A MEASUREMENTS IN THE 7-13 $\mu\text{m}$ WINDOW DURING STS-39

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The spectral and spatial distributions of the greenhouse gas infrared emissions are measured by the CIRRUS 1A (Cryogenic Infrared Radiance Instrumentation for Shuttle) interferometer sensor during STS-39 flight (28 Apr - 6 May, 1991). The spectra in the important 7-11  $\mu\text{m}$  infrared window were recorded. High resolution spectral scans (-1.5  $\text{cm}^{-1}$  instrument resolution) and FASCOD-3 with HITRAN92 database and NMC temperature and pressure profiles are used in an onion peel routine to retrieve gas concentrations from absolutely calibrated radiance data. Scan to scan and profile to profile variability are compared to show the measurement capability of the cryogenic infrared interferometer. The local aerosol is estimated by comparing the modelled and measured CO<sub>2</sub> hot band (10.5  $\mu\text{m}$ ) spectra. The results of concentration profiles retrieved from the spectra (42° south latitude 32° west longitude, local time of 22.4 hr.) are shown. Profiles of CFC-11, CFC-12, HNO<sub>3</sub>, O<sub>3</sub>, and CH<sub>4</sub> developed in this fashion and at different locations are compared with ATMOS (Atmospheric Trace Molecule Spectroscopy), LIMS (Limb Infrared Monitor of the Stratosphere), and situ mean data for these gases.

**INDIRECT GLOBAL WARMING EFFECTS OF TROPOSPHERIC OZONE  
INDUCED BY SURFACE METHANE EMISSION**

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Changing concentrations of atmospheric methane can significantly affect the concentration and distribution of ozone in the troposphere and stratosphere. Changes in the concentrations of these gases can thus influence the radiative forcing on climate. In this study we determine the indirect, time-varying tropospheric radiative forcing and Global Warning Potential (GWP) of  $O_3$  due to an impulse of  $CH_4$  that is equivalent to 36 percent of the atmospheric mass of  $CH_4$ . The direct  $CH_4$  radiative forcing and GWP are also calculated. The LLNL 2-D radiation-chemistry-transport code is used to evaluate the resulting changes in the  $O_3$  and  $CH_4$  atmospheric profiles as a function of time. A correlated k-distribution radiative transfer model is used to calculate the radiative forcing at the tropopause of the globally-averaged atmosphere profiles. The  $O_3$  indirect GWPs vary from ~ 25 after 20 yr integration to ~3 after 500 years. The direct  $CH_4$  GWP vary from ~48 at 20 yrs to ~ 6 at 500 yrs. The 20 year direct  $CH_4$  GWP is ~20% larger than previous estimates due to an increased  $CH_4$  lifetime resulting from the applied impulse. Estimates are made of latitude effects in the radiative forcing calculations.